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MULTICOMPONENT DISTILLATION COLUMNS
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DATED *12th Feb*.....1985

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DYNAMIC SIMULATION OF MULTICOMPONENT DISTILLATION COLUMNS

by



TONY T. WONG

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH
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DEPARTMENT OF CHEMICAL ENGINEERING

EDMONTON, ALBERTA

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THE UNIVERSITY OF ALBERTA
FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled DYNAMIC SIMULATION OF MULTICOMPONENT DISTILLATION COLUMNS submitted by TONY T. WONG in partial fulfilment of the requirements for the degree of MASTER OF SCIENCE IN CHEMICAL ENGINEERING.

Abstract

A model that describes unsteady state multicomponent distillation is developed. The model is free of commonly made assumptions such as constant heat input rate, heat loss rate, tray efficiencies, tray pressures and holdups. Open loop and closed loop simulation for several distillation columns have been performed by use of an Amdahl 5860 computer or an FPS-164 Attached Processor. Open loop simulation involves step changes in feed composition, feed flow, reboiler heat input and reflux flow. Closed loop simulation involves single loop servo control of tray temperature cascaded, using a proportional plus integral controller to the reboiler heat input, and regulatory control of liquid levels for heat input disturbances.

The columns range from a pilot scale water-methanol distillation column to a 29 tray, 5 component hydrocarbon separator to a 75 tray, 10 component industrial separation unit. The simulations were found to be accurate over a wide range of column conditions, and the model was able to obtain solutions for the industrial separator which presents convergence problem in some other simulators.

A semi-implicit Runge-Kutta integration method with self-adjusting parameters is used to solve the nonlinear ordinary differential equations that form the basis of the model. The technique of using this integration method for distillation simulation is discussed. The integration method is shown to be more efficient than conventional

semi-implicit Runge-Kutta techniques, and can be readily applied to distillation problems. The method also offers the advantage of smaller memory requirement over multi-step methods.

The Wilson equation, incorporated with a simplified equilibrium model is shown to be accurate in representing non-ideal liquid vapor equilibria at atmospheric pressures. More rigorous modelling of the equilibria is found to be unnecessary since the results calculated with this model have insignificant differences from the results of the more rigorous model, as shown by the steady state solution.

The simulations indicate that under certain operating conditions, the dynamic response of some variables may exhibit nonminimum phase behavior. The results of this work support past simulation results that inverse response behavior is a common characteristics of the distillation process.

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List of Symbols

A	area of heat transfer to the environment of a stage.
A	Antoine coefficient.
a	Wilson binary interaction energy.
Ar	area of heat transfer in a reboiler.
A _t	effective area of a tray.
B	Antoine coefficient.
C	the total number of components.
C	Antoine coefficient.
c	a measured variable in a control loop.
C _p	heat capacity.
D	distillate molar flow rate.
e	the error term in a feedback control loop.
F	molar flow rate of feed.
f	in a differential equation, $f = dy/dx$.
G	Wilson parameter.
g	an arbitrary scalar function.
g	a first derivative of g.
H	vapor enthalpy.
h	integration time step.
h	liquid enthalpy.
hw	height of weir.
h _t	liquid crest height on a weir.
<u>I</u>	identity matrix.
I	integration error in a PID controller.
<u>J</u>	Jacobian.
K	K value in phase equilibrium.

k incremental function of a difference equation.
 K_i reset rate in a control loop.
 K_p proportional gain in a control loop.
 L liquid molar flow rate.
 M Molar holdup.
 n the total number of stages.
 P pressure
 p output from a controller.
 Q heat flow rate.
 Q_c rate of heat exchange at the condenser stage.
 Q_r rate of heat exchange at the reboiler stage.
 q volumetric flow rate of a stream.
 R ideal gas constant.
 r the set point of a controller.
 S molar flow rate of a vapor side draw.
 s molar flow rate of a liquid side draw.
 T temperature.
 t time.
 U overall heat transfer coefficient.
 V vapor molar flow rate.
 W effective weir width.
 x mole fraction of a component in liquid phase.
 y mole fraction of a component in vapor phase.
 $\hat{y}$ mole fraction of a component in the vapor phase in equilibrium with the liquid phase.
 z mole fraction of a component in the feed stream.
 z liquid level.

Greek Symbols

γ	characteristic root of a difference equation.
γ	activity coefficient.
E_m	Murphree tray efficiency.
ϵ	volume fraction of bubbles in liquid phase.
λ	eigenvalue of a differential equation.
σ	control parameter for local truncation error.
v	molar volume of a component in its pure state.
$\hat{\phi}_i$	vapor fugacity coefficient of a component in a mixture.
ϕ_i^s	liquid fugacity coefficient of a component in its pure state.
T	ambient temperature.
τ	reset time of a controller, $\tau = 1/K_i$.

Subscripts

f	a property of a feed stream.
i	a property of component i .
j	a quantity associated with stage j .
n	a quantity associated with the bottom stage.
s	a quantity associated with a stiff variable.
st	a property of the input steam.

Superscripts

s	thermodynamic property of a component in its pure saturated state.
n	time step.
$'$	bias term in a control loop.

- " set point of a control loop.
- ∞ a quantity taken to the limit as $t \rightarrow \infty$.

Note

- a vector is denoted by a symbol in bold type.
- a matrix is denoted by a "_" beneath the symbol.
- an averaged quantity is denoted by a "-" on top of the symbol.
- the derivative of a vector function is denoted by a "." on top of the symbol.

1. Introduction

As distillation forms an important process in the production line of most chemical plants, it is of economical interest to achieve satisfactory control of distillation columns. Many advanced control strategies are available to improve the control of distillation columns, but in order to apply these control schemes properly, it is important to understand the dynamic behavior of the columns. Since actual plant data are often expensive and difficult to collect, it is more desirable to perform computer simulation using a reliable model. It is the primary objective of this study to develop such a model and evaluate its accuracy with available data.

The dynamic behavior of distillation columns can be rigorously described by sets of ordinary differential and algebraic equations as described by Rademaker et al(1). The correct formulation of such systems of equations was known long before digital computers were available to obtain a solution to the system of equations. However, it was not until the vast improvement in digital computer technology over the past two decades, that rigorous plate-to-plate calculation of distillation columns became feasible. Without the power of modern digital computers, analysis was limited to linearized models, for columns with a small number of trays, often only for binary mixtures and the means of computation was usually analog or hybrid computers. Stojak(2) concluded from a simulation study of a crude oil

distillation unit in 1973 that for distillation process simulation, modern hybrid computation provides a marginal speed advantage to third generation digital computers, but program development time is much greater than for digital computation. It is generally considered that the rapid development of high speed digital computers could easily defeat the use of a hybrid computer for this type of problem.

In recent years considerable effort has been spent on the simulation of the dynamics of multicomponent distillation columns using high speed digital computers. Early contributions included that of Peiser and Grover(3), in which a dynamic model of a multicomponent distillation tower was developed based on energy and mass balances and tray hydraulics. The model was applied to solve a plant problem involving flooding in the trays near the bottom of the tower. Waggoner and Holland(4) developed a column model using a similar approach for the simulation of the dynamic behavior of complex distillation columns. A generalized model that takes into account the effects of the hydraulics and mixing on the trays was presented by Tetlow et al(5). However, the θ method of convergence used by Holland and co-workers(20,33) to solve the unsteady state equations is iterative and is relatively inefficient for the large number of equations present in the system. More recent work included that of Howard(5), in which a general model was developed with the basic column equations to allow the

specification of variable plate holdups, variable plate efficiencies, heat loss from the column and finite time liquid flow dynamics. Using a method to find the implicit variables independent of the numerical methods, Howard proceeded to solve a distillation problem involving a 14 tray column operated at total reflux with a mixture of benzene, toluene and ethylbenzene. The explicit Kutta-Merson integration method was used, although the method is only conditionally stable, so relatively small integration time steps were used to ensure stable solution. In a subsequent study, Howard(6) compared the simulated results to the experimental data obtained from an existing column and concluded that inadequate information about the characteristics of the real column caused more errors in the simulation results than the deficiencies in the generalized computer model did. The basic mathematical model used by these authors forms the basis for most models that are developed.

On the other hand, Economopoulos(8) developed a mathematical model based on "isovrastic" units and a solution method which is expected to be easier and more stable than those reported in the literature. The author used this method to simulate the open loop and closed loop behavior of a pilot scale extractive distillation unit with a feed mixture composed of n-butyl acetate, acetic acid and water. A feed forward control scheme was proposed based on the simulation results which showed significant improvement

in the quality control of the products using the new control scheme. Morris and Svrcek(9), in response to the inability of conventional equilibrium models to handle absorbing and stripping problems, developed a distillation tray model based on a mass transfer approach. The model was tested with data obtained from a 75 stage industrial distillation unit, but the general application of this model to other columns still requires a prior knowledge of the mass transfer characteristics of the components. To reduce the enormous dimensionality of the process model associated with the simulation of trains of distillation columns so that computer simulation can be feasible, Cho et al(10) proposed a reduced order dynamic model which approximates the composition and flow profiles in sections of a column by polynomials. Orthogonal collation was used to approximate the partial difference equation and a semi-implicit Runge-Kutta method proposed by Ballard et al(11) was utilized to integrate the transient equations. However, the simulations carried out to demonstrate the use of the method are only concerned with single columns of relatively small scale.

Most published results on column simulation in the literature do not contain sufficient details to allow duplication or continued investigation. Among the exceptions are the collection of simulation results compiled by Holland and Liapis(12) and the simulation study of an extractive distillation column by Gallun(13), in which

Gear's algorithm is applied with the utilization of the Kubicek algorithm for efficient solution of banded sparse matrices. All this work fully demonstrated that the utilization of digital computers in process simulation is not only economically viable, it also makes possible the simulation of columns with a high degree of complexity and the flexible use of a large range of solution methods.

A number of different numerical methods and solution procedures have been used over the years for the solution of the stiff system of equations that often arises in column simulation. For stability considerations, most methods are implicit and are often incorporated with some selection scheme for integration time steps for better efficiency. Among the various integration methods available, the semi-implicit Runge-Kutta (SIRK) method has gained much popularity over the last few years. The family of SIRK methods was first investigated by Rosenbrock(14). Since then, the potential of this method in solving stiff systems of differential equations has prompted a number of researchers to improve the accuracy and efficiency of the method. Caillaud and Padmanabhan(15) presented a third order method which has absolute stability characteristics, and compared the solutions for a few linear and nonlinear problems obtained by this method to the solution of other existing SIRK methods. Cash(16) developed a second order method and a third order method from which an estimate of the local truncation error can easily be obtained, so that

it is possible to adjust the integration step size. A more detailed analysis of the techniques available to obtain estimates of the local truncation error for different SIRK methods has been given by Chan and co-workers(17).

Michelsen(18) modified the SIRK method by Caillaud and Padmanabhan(15) to obtain an algorithm that uses a full step/half-step technique to facilitate flexible adjustment of the step size. Ballard et al(11) pioneered the application of this method to the solution of distillation problems. The method employed by Ballard et al(11) uses a splitting technique to simplify the computation of the Jacobian matrix. An integration method which recently appeared in the literature is the adaptive SIRK (ASIRK) method developed by Prokopakis(19,20). In a few numerical examples presented by Prokopakis, this method was shown to perform better with Gear's algorithm and some of the other SIRK methods.

Another subject of equal importance in distillation simulation is the accurate prediction of phase equilibria. A number of phase equilibrium models have been developed over the years to describe systems under a broad range of physical conditions and thermodynamic characteristics. The most active research today is still in the areas concerning nonideal phase equilibria. Although it is beyond the scope of this work to review past achievements, some insights can be given concerning the representation of two phase equilibria under pressures close to atmospheric, which is

the case for all of the simulations studies included in this work. The most difficult problem in vapor-liquid equilibrium calculations often lies in the ability to accurately represent the excess Gibbs free energy as a function of temperature and composition for an enormous variety of liquid solutions. Several versions of the integral form of the excess Gibbs free energy function have been introduced over the years. These versions are exemplified by the Van Laar equation and the Margulus equation which are somewhat difficult to extend for systems having more than two components, and the more sophisticated NRTL equation which can predict the formation of a second liquid phase, but requires more parameters. The Wilson equation(21) which has recently received considerable attention requires only two temperature independent parameters obtained from experimental measurement of binary mixtures, and is flexible enough to be generalized for multicomponent systems. Hakim(22) and Gallun(13) have used the equation for column simulations with satisfactory results. For these reasons the Wilson equation can be used when high accuracy is not required, or in situations where more reliable information on the phase equilibria of a system is not available, as in some cases considered in this work.

Based on a mathematical model of a distillation column, and the solution procedure of the ASIRK method, a computer program was developed in this study to perform simulation of

the steady state and dynamic behavior of several distillation columns. Being highly nonlinear, the dynamics of distillation columns often exhibits interesting behavior which poses challenging problems to process control engineers. Some nonlinear behavior has been reported in the literature, and the especially interesting aspects of such dynamics are the inverse response behavior and the asymmetric response time for different disturbances. Some of the more detailed studies are those of Waller(23) and Luyben(24) for binary columns, Stathaki and et al(25,26) on an industrial column. The dynamic simulator developed during the course of this study becomes a convenient and useful tool to investigate this nonlinear behavior.

In Chapter 2, a formal treatment of the basic model is given for a generalized distillation column. As the model gives rise to sets of nonlinear ordinary differential equations and nonlinear algebraic equations, the numerical procedures employed to solve these equations are discussed in Chapter 3. A numerical example is given in Chapter 3 to illustrate the performance of the ASIRK method in solving equations describing a simple hydrocarbon separator.

In Chapter 4, the results of simulating a five component hydrocarbon separator with inverse response behavior are presented. The simulation is for disturbances in the feed flow rate, heat input rate and reflux flow rate of various magnitudes.

Chapter 5 deals with the simulation of the dynamic behavior of a water-methanol binary column. Transient experimental response data from the column(3) is compared to the model predictions for feed rate changes. Based on the comparison, refinements to the basic model established in Chapter 2 are made so that the model predictions can provide satisfactory representation of the true behavior of the column.

Chapter 6 is concerned with the modelling of the extractive distillation column studied by Gallun(13). A model for the control system is developed and simulation is performed for heat input changes and temperature set point changes. The formulation of the controller equations to be incorporated into the single step method of ASIRK is presented and the simulation results are discussed.

Some preliminary simulation results for an industrial distillation unit are presented in Chapter 7. The simulation study illustrates the feasibility of computer simulation of large scale distillation columns even with highly nonideal chemical components.

i.

2. Column Dynamic Model

2.1 Introduction

In a distillation process, liquid and vapor flowing countercurrently come into continuous contact on a series of trays. The complexity of the process can range from a simple column with a single feed and two product streams, to a complex column with multiple feed streams, multiple side stream products, and nonideal reacting chemical species on all trays. The rigorous modelling of such process requires the simultaneous treatment of the material balance equation and the energy balance equation.

In this chapter, the modelling equations for a generalized tray are presented. These equations are easily extended for a series of trays to describe a complete distillation column. The equations can also be modified to model units such as condensers and reboilers. These equations form the basis of a dynamic simulator which can be implemented in a digital computer for simulating the dynamic behavior of distillation columns.

2.2 Formulation of the Tray Model

To model a distillation column, it is convenient to consider the column consisting of a series of stages which include the condenser and reboiler. Obviously, the condenser and the reboiler are separate units and in fact are not even necessarily in close proximity to the column.

However, for digital computer solution, it is convenient to consider the condenser and reboiler as simply two stages of an n stage process. In this study, the designation of stage number starts from the top, so the condenser stage will be considered stage 1 while the reboiler is stage n . The liquid and vapor streams are numbered with respect to their origin. For example, the rate of the liquid overflow from stage j is defined as L_j and the rate of the vapor stream leaving stage j is denoted by V_j .

Figure 2.1 shows schematically the process on the j th stage. The stage receives an external feed, liquid from the stage above through the downcomer, and a vapor stream from the stage below. The liquid on the stage overflows to the stage below and the vapor from the tray flows to the stage above. The general tray model also allows for the withdrawal of liquid and vapor from the tray as products and for heat to be exchanged either with the environment or with an external device.

In the following sections, a mathematical model to describe this process is discussed in detail. Only the final form of the equations are presented with the detailed derivations given in Appendix A.

2.2.1 Tray Material Balance

In deriving the total and component material balance equations for stage j , the following assumptions are made

- ii. the mixture is not chemically reactive;

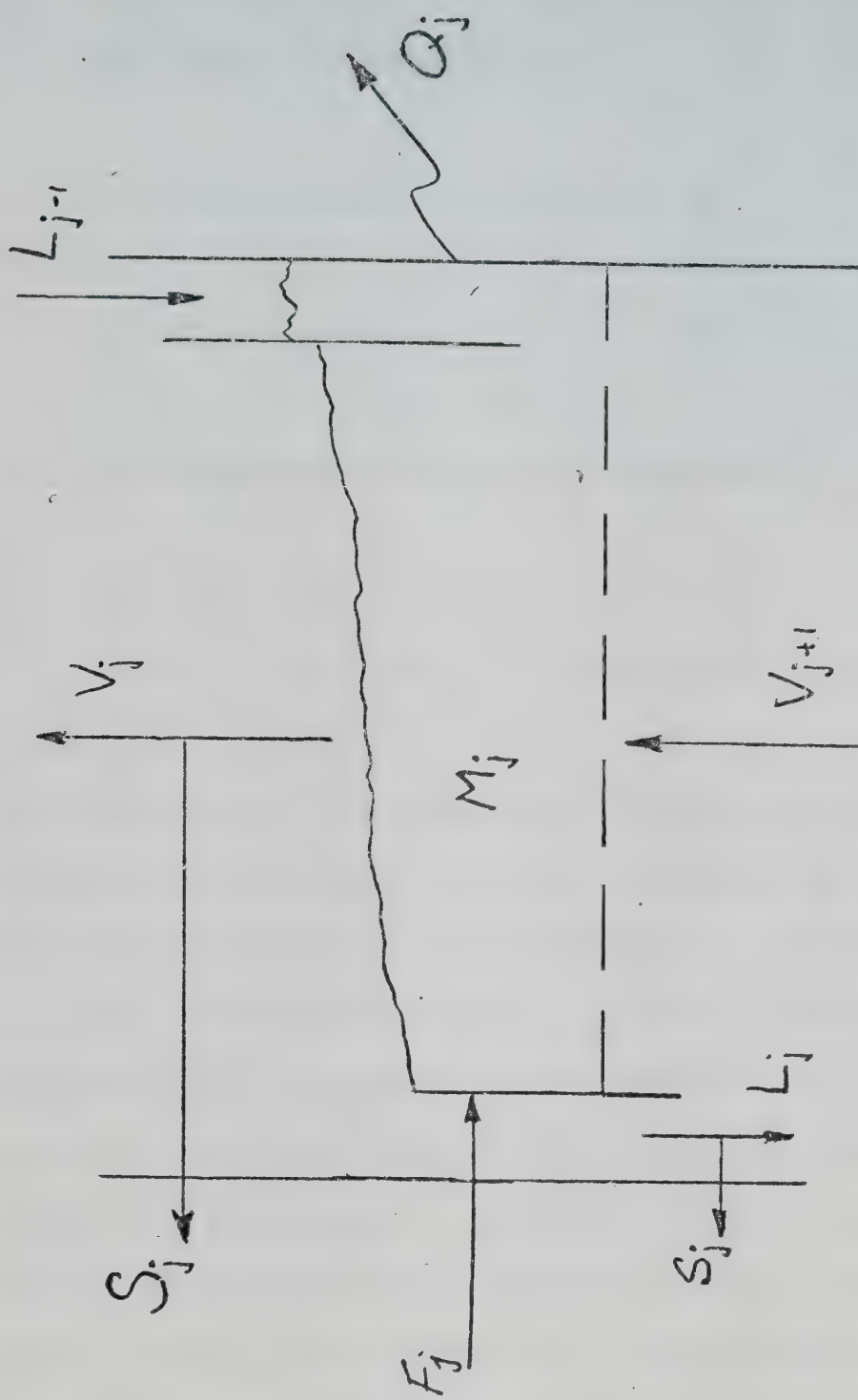


Figure 2.1 Schematic Diagram of a Generalized Tray

- iii. the liquid on the tray is perfectly mixed;
- iv. material storage in the vapor phase and in the downcomer is negligible.

The mass balance on the tray is

$$dM_j/dt = F_j + V_{j+1} + L_{j-1} - (V_j + S_j) - (L_j + s_j) \quad (2.1)$$

and the component balance for component i becomes

$$\begin{aligned} dx_{ji}/dt = & \{F_j(z_{ji} - x_{ji}) + V_{j+1}(y_{j+1,i} - x_{ji}) \\ & + L_{j-1}(x_{j-1,i} - x_{ji}) - (V_j + S_j)(y_{ji} - x_{ji})\} / M_j \end{aligned} \quad (2.2)$$

For simplicity, the subscript " i " will be dropped in equations concerning component balance in this chapter and also in Appendix A. The composition variables, x_{ji} , y_{ji} and z_{ji} , will be replaced by x_j , y_j and z_j respectively to represent the composition of component i on stage j . Note that the heat exchange on the stage, Q_j , has no direct effect on the material balance, but the effect will be reflected through the variation in the liquid and vapor flow rates. This can be seen from consideration of the energy balance, which is discussed in a later section in this chapter.

2.2.2 Tray Energy Balance

In deriving the energy balance, several simplifying assumptions are made

- i. energy and material storage in the vapor phase is negligible;
- ii. energy storage in the tray metal is negligible;
- iii. energy storage in the downcomer is negligible, and
- iv. the heat of mixing among the chemical species is negligible.

Assumption (i) is generally valid when the pressure inside the column is low and the vapor density is small. This assumption, however, has to be applied with caution for simulating the behavior of high pressure systems. For assumption (ii), Simonsmeier(29) concluded from a study of the modelling of a binary column that the inclusion of energy storage in the tray metal only gave marginally slower overall dynamics. Assumption (iv) is even true in most chemical systems since the dominant heat effect in distillation processes is due to the vaporization and condensation of fluids, which usually involves a much larger amount of heat exchange than the heat of mixing.

An energy balance on stage j using the assumptions above can be stated as

$$\begin{aligned} d[M_j h_j]/dt = & \{F_j(h_{f,j}) + Q_j + V_{j+1}H_{j+1} + L_{j-1}h_{j-1} \\ & - (V_j + S_j)H_j - (L_j + s_j)h_j\} \end{aligned} \quad (2.3)$$

and by the use of the total mass balance equation, the following expression, as established in Appendix A, is obtained

$$\begin{aligned} dh_j/dt = \{ [F_j(h_{j+1}-h_j)] + Q_j + V_{j+1}(H_{j+1}-h_j) \\ + L_{j-1}(h_{j-1}-h_j) - (V_j+S_j)(H_j-h_j) \} / M_j \end{aligned} \quad (2.4)$$

Following the procedure used by Brosilow et al(28), equation 2.4 is transform into a linear algebraic equation of the form

$$E_j = -a_j L_{j-1} + \beta_j V_j - \psi_j V_{j+1} \quad (2.5)$$

The derivation of equation 2.5 and the definition of the terms E_j , a_j , β_j and ψ_j are also given in Appendix A.

2.2.3 Equilibrium Model

For a homogeneous chemical mixture at low to moderate pressures, the equilibrium relationship for component i is

$$y_i \hat{\phi}_i P = x_i \gamma_i P_i^s \phi_i^s \quad (2.6)$$

Even though $\hat{\phi}_i$ and ϕ_i^s deviate from unity as pressure increases, the difference is usually insignificant and the ratio of the values is very close to unity, therefore in equation 2.6 their effect tends to cancel out. Thus as an approximation, equation 2.6 can be written as

$$y_i P = x_i \gamma_i P_i^s \quad (2.7)$$

The equilibrium relationship above is suitable for miscible chemical systems at low pressures. The model can be extended to higher pressures without much difficulty if the variations in the fugacity coefficients are accounted for by some thermodynamic model. However, to keep the model in a simple and still usable form, equation 2.7 was adopted for the simulation study.

It is common in the petrochemical industry to define the equilibrium ratio of component i as

$$K_i = \frac{y_i}{x_i} \quad (2.8)$$

Thus from the equilibrium model

$$K_i = \frac{\gamma_i P_i^s}{P} \quad (2.9)$$

and K_i is called the "K value of component i ". To calculate the K value, the activity coefficient and the vapor pressure at the system pressure, temperature and composition must be known. Numerous correlations have been used throughout the years with varying degree of success. In this simulation study, an equation introduced by Wilson(21) is used for calculating the activity coefficient of component i in nonideal liquid mixtures

$$\ln(\gamma_i) = 1 - \ln \sum_j \{x_j G_{ij} - \frac{\sum_k [x_k G_{ki}]}{\sum_j (x_j G_{kj})}\} \quad (2.10)$$

where $G_{ij} = v_j/v_i \exp\{-a_{ij}/RT\}$

In equation 2.10, all summations are over all species. The interaction energy a_{ij} is assumed to be independent of temperature and composition, and is treated as a true constant. An important advantage in using the Wilson equation is that the values for a_{ij} can be obtained from experiments involving binary mixtures at a single temperature, and yet the equation can be applied to multicomponent systems over a wide range of temperature.

To calculate the vapor pressure of component i , the commonly used Antoine equation was chosen for the simulations

$$\ln(P_i^s) = A_i - \frac{B_i}{T+C_i} \quad (2.11)$$

For hydrocarbon systems, deviation from ideality in the liquid phase is often insignificant. Therefore the use of the Wilson equation is not necessary. For such systems, it is common in the literature to correlate the K value empirically by means of polynomials or some simple function of temperature and pressure.

Tray efficiency is a measure of the approach to equilibrium of the liquid and vapor on a tray. For the

simulation of the dynamic behavior of columns, the vapor compositions on each tray have to be adjusted with the tray efficiency. The Murphree tray efficiency, which is the bulk efficiency of the entire tray, is defined as

$$E_m = \frac{(y_{ji} - y_{j+1i})}{(\hat{y}_{ji} - y_{j+1i})} \quad (2.12)$$

where $\hat{y}_{ji}$ is the vapor composition of component i in equilibrium with the liquid on the j th stage.

Based on the above equilibrium model, the equilibrium temperature of the mixture can be established via a bubble point calculation. Given the stage pressure and the composition of the liquid, the equilibrium temperature is such that the sum of the mole fractions in the vapor phase is unity, that is

$$\sum_i y_i \{T, P, x\} = 1 \quad i=1, 2, \dots, C \quad (2.13)$$

This physical constraint has to be met at every time step of the computer solution in order to satisfy the equilibrium condition.

2.2.4 Tray Holdup

Equation 2.5 alone cannot be used to solve for the liquid and vapor flow rates inside the column since for an n stage tower, there are n liquid streams and n vapor streams (ie. $2*n$ equations) while there are only n energy balance

equations. However the mass balance equation can be used to satisfy the remaining degree of freedom. Two different approaches have been used in this study

- i. mass balance based on constant tray holdup;
- ii. mass balance based on tray holdup as a function of liquid flow rates.

For the first case, equation 2.1 becomes an algebraic equation since the left hand side of the equation equals zero, and equation 2.1 can be written as

$$m_j = L_{j-1} - L_j - V_j + V_{j+1} \quad (2.14)$$

where $m_j = S_j + s_j - F_j$. Recalling the energy balance equation

$$E_j = -a_j L_{j-1} + \beta_j V_j - \psi_j V_{j+1} \quad (2.5)$$

Equations 2.14 and 2.5 can be solved simultaneously to obtain the liquid and vapor flow rates. Details of the solution procedure can be found in Appendix A.

For the second case, the Francis weir formula(13) was used to correlate the liquid flow rate with the tray holdup. The weir equation used is developed in Appendix A, that is

$$M_j = \{0.04347[L_j v_j / W]^{2/3} + hw\} A_t (1-\epsilon) / v_j \quad (2.15)$$

with v_j in kmol/m^3 , A_t in m^2 , W and hw in metres. Thus,

$$\frac{dL_j}{dM_j} = \left\{ \frac{W}{0.02898 A_t (1-\epsilon)} \right\} \left\{ \frac{W}{L_j v_j} \right\}^{-1/3} \quad (2.16)$$

And since

$$dL_j/dt = [dL_j/dM_j] [dM_j/dt] \quad (2.17)$$

substitution of equation 2.1 and equation 2.16 into the right hand side of equation 2.17 yields

$$dL_j/dt = [F_j + V_{j+1} + L_{j-1} - (V_j + S_j) - (L_j + s_j)] \left\{ \frac{W}{0.02898 A_t (1-\epsilon)} \right\} \left\{ \frac{W}{L_j v_j} \right\}^{-1/3} \quad (2.18)$$

The nonlinear ordinary differential equation of the form of Equation 2.18 can be solved numerically for the liquid flow rates. The tray holdup can be calculated from the flow rates by use of equation 2.15 and the vapor flow profile can be solved from the energy balance equation. The procedure for the method of solution is also included in Appendix A.

2.3 Condensers

2.3.1 Total Condenser

The condenser stage and the reboiler stage can be modelled simply as special cases of the general tray equations. For a total condenser, the vapor stream is condensed to liquid by removing heat, and a portion of this condensed liquid (saturated or subcooled) is returned to the column as reflux. Thus,

$$\begin{aligned} L_0 &= 0 \\ V_1 &= 0 \end{aligned} \quad (2.19)$$

So the distillate in such case may be considered as a liquid sidestream draw-off. Therefore the mass balance on stage 1 is written as

$$dM_1/dt = F_1 + V_2 - (L_1 + D) \quad (2.20)$$

Following the same procedure as for the general tray, the component balance for component i (subscript i is omitted for simplicity) on stage 1 becomes

$$dx_1/dt = \{F_1(z_1 - x_1) + V_2(y_2 - x_1)\} \quad (2.21)$$

Equation 2.21 shows that the liquid composition in the condenser is not a direct function of the reflux flow rate,

nor of the distillate flow rate, since if the liquid in the condenser is well mixed, withdrawal of any amount of liquid should not alter the overall composition.

The energy balance for the total condenser, to calculate the condenser heat removal requirement is

$$Q_c = -F_1(h_{f,1} - h_1 - \xi_1^*) + \beta_1 S_1 - \psi V_2 \quad (2.22)$$

where ξ^* and ψ are terms defined in Appendix A. The sign of Q_c is generally negative since heat is removed from the condenser. It should be noted that in writing equation 2.22, it is assumed that the condensed liquid is saturated. Although the liquid may be subcooled, the approximation is reasonable from the energy balance view point, since it is the heat of condensation of the vapor stream that contributes most to the condenser heat load.

2.3.2 Partial Condenser

For a partial condenser, equations 2.1, 2.2 and 2.5 developed for the general tray are applicable since the condenser essentially operates as an equilibrium stage. In this type of condenser, V_1 is the vapor product and L_1 is the reflux, with the condition that

$$L_0 = 0 \quad (2.23)$$

The heat load of a partial condenser, assuming saturated

reflux, is

$$Q_c = -F_1(h_{t,1} - h_1 - \xi_1^*) + \beta_1(V_1 + S_1) - \psi V_2 \quad (2.24)$$

2.4 Reboilers

Similarly, a partial reboiler can be treated as an equilibrium stage with no vapor input. Jacketed reboilers, kettle type reboilers and internal reboilers belong to this category. The applicable condition for this type of reboiler is

$$V_{n+1} = 0 \quad (2.25)$$

and the balance equations 2.1, 2.2 and 2.5 can be applied. The flow rate of the bottoms product is represented by L_n . The rate of heat input to the reboiler is

$$Q_r = -F_n(h_{t,n} - h_n - \xi_n^*) + \beta_n(V_n + S_n) - \alpha_n L_{n-1} \quad (2.26)$$

3. Numerical Techniques for the Dynamic Simulation

The distillation column mathematical model developed in Chapter 2 involves large sets of nonlinear ordinary differential equations and nonlinear algebraic equations. For a numerical solution of these equations to be feasible in terms of the use of computing resources, it is necessary to employ efficient numerical algorithms which give reasonably accurate results. In this simulation study, some numerical methods considered to be efficient have been used to solve the large number of simultaneous equations. This chapter illustrates how these numerical methods are adapted to the modelling equations with an emphasis on the formulation of computer algorithms.

3.1 Solution Method for a Nonlinear Algebraic Equation

The need to solve nonlinear algebraic equations in distillation simulations arises from the equilibrium calculation on each stage. Given the pressure and the liquid composition of a particular stage, the stage temperature must be computed iteratively to satisfy equation 2.12, that is to solve the expression

$$g(T) = \sum_i K_i x_i - 1 = 0 \quad i=1,2,\dots,C \quad (3.1)$$

for the equilibrium temperature so that the sum of the vapor mole fractions equal unity. Since the solution of equation 3.1 does not depend on the temperature of any other

stages, the equation can be solved using Newton's method for a single equation expressed as

$$T_{k+1} = T_k - g(T_k)/g'(T_k) \quad (3.2)$$

Newton's method is especially suitable for computer solution because it requires only an initial temperature to start the iteration and has a quadratic rate of convergence. For computer solution, the derivative $g'(T)$ is not represented by an analytical expression but by a forward difference approximation. Since the analytical form of $g(T)$ can be quite different for different equilibrium models and is generally a complicated function to evaluate, use of a numerical approximation has the advantage of model independence and simplicity.

3.2 Solution Method for a System of Linear Algebraic Equations

Large sets of algebraic equations must be solved at each time step of the simulation because of the implicit integration algorithm which will be discussed in the following sections. For a distillation column with no pump-arounds, the coefficient matrix of these algebraic equations is tridiagonal in structure and the system of equations can be solved very efficiently with the Thomas algorithm. Suppose the system of equations

$$\underline{M}_{m \times m} \underline{x}_{m \times 1} = \underline{d}_{m \times 1} \quad (3.3)$$

has a tridiagonal coefficient matrix $\underline{M}$ with

diagonal elements $b_j \quad j = 1, \dots, m$

lower diagonal elements $a_j \quad j = 2, \dots, m$, and

upper diagonal elements $c_j \quad j = 1, \dots, m-1$

The Thomas algorithm solves the equations directly as follows

$$\beta_1 = b_1$$

$$\gamma_1 = d_1 / \beta_1$$

$$\beta_j = b_j - (a_j c_{j-1}) / \beta_{j-1} \quad j = 2, \dots, m$$

$$\gamma_j = (d_j - a_j \gamma_{j-1}) / \beta_j \quad j = 2, \dots, m$$

and

$$x_n = \gamma_n$$

$$x_j = \gamma_j - c_j x_{j+1} / \beta_j \quad j = m-1, \dots, 1$$

3.3 Solution Method for Ordinary Differential Equations

For a system of C components, equation 1.2 gives rise to C sets of simultaneous, nonlinear ordinary differential equations, whose variables often have a large range of response times. Such a system of equations is commonly termed a 'stiff' system(10). For stability reasons, the numerical schemes used for this type of equations are necessarily implicit. The numerical scheme used in this study is the Adaptive Semi-Implicit Runge-Kutta (ASIRK) method developed by Prokopakis(19).

3.3.1 The ASIRK Integration Method

The basic structure of the ASIRK method follows that of the semi-implicit Runge-Kutta formula first proposed by Rosenbrock(14) with two stages

$$y^{n+1} = y^n + w_1 k_1 + w_2 k_2 \quad (3.4)$$

$$\begin{aligned} [I - ha_1 J\{y^n\}] k_1 &= h f\{y^n\} \\ [I - ha_2 J\{y^n + c_1 k_1\}] k_2 &= h f\{y^n + b k_1\} \end{aligned} \quad (3.5)$$

where $y^n = y(t)$ and $y^{n+1} = y(t+h)$. The characteristic root of the above difference equation is

$$\gamma = \frac{\{1 + [w_1 + w_2 - (a_1 + a_2)]h\lambda + [a_1 a_2 - (w_1 a_2 + w_2 a_1 - w_2 b)](h\lambda)^2\}}{(1 - a_1 h\lambda)(1 - a_2 h\lambda)} \quad (3.6)$$

The parameters w_1, w_2, a_1, a_2, b and c_1 are related by the following formulae to facilitate third order accuracy

$$\text{1st order:} \quad w_1 + w_2 = 1 \quad (3.7)$$

$$\text{2nd order:} \quad w_1 a_1 + w_2 a_2 + w_2 b = 1/2 \quad (3.8)$$

$$\text{3rd order:} \quad w_1 a_1^2 + w_2 a_2^2 + w_2 b(a_1 + a_2) = 1/6 \quad (3.9)$$

$$\text{3rd order:} \quad w_2(a_2 c_1 + b^2/2) = 1/6 \quad (3.10)$$

There are six unknown parameters and only four equations.

Rosenbrock(14) selected the following set of parameters

$$w_1 = -0.413 \quad w_2 = 1.413$$

$$a_1 = 1.408 \quad a_2 = 0.592$$

$$b = c_1 = 0.174$$

Prokopakis(19) modified the above method by specifying $a_1 = a_2 = a$ and $c_1 = 0$, so the resulting equations become

$$y^{n+1} = y^n + w_1 k_1 + w_2 k_2 \quad (3.11)$$

$$[I - haJ\{y^n\}] k_1 = h f\{y^n\}$$

$$[I - haJ\{y^n\}] k_2 = h f\{y^n + bk_1\} \quad (3.12)$$

This modified form requires only one evaluation of the Jacobian matrix, and one matrix inversion for the expression enclosed in the square brackets.

With the above modifications Prokopakis(19) constructed a second order semi-implicit Runge-Kutta method. In order to have second order accuracy, equations 3.7 and 3.8 must be satisfied. Equation 3.10 for third order accuracy is also included to improve the order of accuracy. Equation 3.6, taking to the limit as $(h\lambda)$ approaches infinity, yields the fourth equation that ties the yet undetermined parameters together. With these four equations (3.6, 3.7, 3.8 and 3.10) there are a total of five unknown parameters, namely a , b , w_1 , w_2 and γ^∞ , where γ^∞ denotes $\gamma\{h\lambda \rightarrow \infty\}$. These equations are then rearranged into the following form:

$$a = \frac{1 + [1 - (1 - \gamma^\infty)/2]^{1/2}}{1 - \gamma^\infty} \quad (3.13)$$

$$b = [3(0.5-a)]^{-1} \quad (3.14)$$

$$w_2 = 3(0.5-a)^2 \quad (3.15)$$

$$w_1 = 1 - w_2 \quad (3.16)$$

Since equation 3.9 is not satisfied, the method remains second order in principle.

Equations 3.13 to 3.16 represent four independent equations and five unknowns (γ^∞ , a , b , w_1 and w_2), so one degree of freedom remains. A feature of the ASIRK solution method is the selection, or adaption of γ^∞ at each time step such that the accuracy of the method is optimized.

In the development of the adaptive algorithm, Prokopakis(19) introduced the pseudo-eigenvalue of the stiff variable. With the stiff variable identified as the variable having the largest rate of change during the last time step, the pseudo-eigenvalue of the stiff variable can be obtained conveniently by the first order approximation

$$\lambda_s = \frac{1 - h[f_s\{y^n\}/k_{1s}]}{ha} \quad (3.17)$$

or the second order approximation

$$\lambda_s = \frac{1 - h \frac{w_1 f_s\{y^n\} + w_2 f_s\{y^n + bk_1\}}{w_1 k_{1s} + w_2 k_{2s}}}{ha} \quad (3.18)$$

Prokopakis nevertheless recommended the use of equation 3.18 for its higher accuracy.

From an analysis of the homogeneous solution of a linear first order ordinary differential equation(9,10), it is observed that the characteristic roots of difference equations (such as the Runge-Kutta methods) intersect with the characteristic root corresponding to the exact solution of the ordinary differential equation at different values of $h\lambda$. At the point of intersection, the particular difference equation will provide the best approximation of the exact solution. Since each difference equation can be characterized by a unique value of γ^∞ , it is possible to fit the points of intersection as a function of $h\lambda$ with an empirical formula such as

$$\gamma^\infty = \frac{A}{B + (h\lambda_s)^2} + \frac{C}{D + h\lambda_s} + E \quad (3.19)$$

where the numerical value of the fitting parameters are given(9) as

$$A = -4.9221$$

$$B = 21.1642$$

$$C = 0.5287$$

$$D = -0.6889$$

$$E = 0.0$$

Note that in equation 3.19 the pseudo-eigenvalue of the stiff variable is used in the correlation to emphasize

tracking of the stiff variable.

Starting with an initial value of γ^∞ (or the value from the last time step), the parameters of the ASIRK are determined by equations 3.13 to 3.16. The parameters are used to obtain the new solution vector y^{n+1} , from which a stiff variable can be identified. The pseudo-eigenvalue of the stiff variable is then approximated by either equation 3.17 or 3.18 and a new γ^∞ can be calculated with equation 3.19. With this updated value of γ^∞ a new set of parameters can be obtained from equations 3.13 to 3.16 and the iterative process carried out continuously.

3.3.2 Step Size Control

Along with the adaptive scheme, Prokopakis and Seider(20) also proposed a rather sophisticated step size control algorithm which requires the solution of a fourth order polynomial. In this study, a simpler approach suggested by Ballard et al(11) was employed since the maximum integration step size for the column control system in the simulations will be limited by the control system sample time interval, which will be at most a few minutes. Therefore time step control will not yield a significant saving in computational cost except at the beginning of the transient where the variables are changing rapidly. The simple formula for time step control is selected as

$$h^{n+1} = h^n [\sigma/e_t]^{0.5} \quad (3.20)$$

with limits $0.25 \leq h^{n+1}/h^n \leq 2.0$

where σ is a user specified error control parameter.

3.3.3 Application of the ASIRK Method for Column Simulation

The component balance represented by equation 2.2 forms a set of nonlinear ordinary differential equations for the i th component on different stages, and the j th element of the derivative vector is expressed as

$$\begin{aligned} f\{x_j\} = & \{F_j(z_j - x_j) + V_{j+1}(y_{j+1} - x_j) \\ & + L_{j-1}(x_{j-1} - x_j) - (V_j + S_j)(y_j - x_j)\} / M_j \end{aligned} \quad (3.21)$$

$j = 1, 2, \dots, n$

The elements of the Jacobian matrix are defined as

$$J_{mn} = [\partial f\{x_m\} / \partial x_n] \quad (3.22)$$

and since the compositions on the j th stage are only influenced by those of the adjacent stages, the Jacobian becomes a tridiagonal matrix with diagonal elements

$$J_{jj} = -[F_j + V_{j+1} + L_{j-1} - (V_j + S_j)(K_j - 1)] / M_j \quad (3.23)$$

The lower diagonal elements can be shown to be

$$J_{j,j-1} = L_{j-1} \quad (3.24)$$

and the upper diagonal elements

$$J_{j,j+1} = V_{j+1}K_{j+1} \quad (3.25)$$

The ASIRK method requires two evaluations of $f(x_j)$ and one evaluation of the Jacobian for each time step. Also the incremental functions k_1 and k_2 have to be calculated by solving systems of linear algebraic equations. Fortunately, because of the structure of the Jacobian, the systems of equations also have a tridiagonal structure and can be solved by the Thomas algorithm.

The tray hydraulics equation

$$\begin{aligned} dL_j/dt = [F_j + V_{j+1} + L_{j-1} - (V_j + S_j) - (L_j + s_j)] \\ * [W_j(0.02898 A_t(1-\epsilon))^{-1} [L_j v_j] W_j]^{1/3} \end{aligned} \quad (2.17)$$

applied for each tray results in another set of nonlinear equations which is solved with the same integration method. For this system of equations, the Jacobian is bidiagonal with non-zero elements on the main diagonal and the lower diagonal only.

3.4 A Numerical Example using the ASIRK

To evaluate the performance of the ASIRK method, the algorithm is used to simulate the dynamic behavior of a simple hydrocarbon distillation column previously simulated by Holland and Liapis(12) using the θ method. The problem

is solved with the ASIRK method and with the constant parameter semi-implicit Runge-Kutta method suggested by Ballard et al(11), abbreviated as the BBSIRK. The formula for this Runge-Kutta method, which is also second order, is

$$\mathbf{y}^{n+1} = \mathbf{y}^n + 2\mathbf{k}_1 - \mathbf{k}_2 \quad (3.26)$$

with incremental functions

$$\begin{aligned} \mathbf{k}_1 &= [\mathbf{I} - h\mathbf{J}\{\mathbf{y}^n\}]^{-1} h\mathbf{f}\{\mathbf{y}^n\} \\ \mathbf{k}_2 &= [\mathbf{I} - 2h\mathbf{J}\{\mathbf{y}^n\}]^{-1} h\mathbf{f}\{\mathbf{y}^n - 0.5\mathbf{k}_1\} \end{aligned} \quad (3.27)$$

and local truncation error estimate of

$$\mathbf{e}_t = \mathbf{k}_2 - \mathbf{k}_1 \quad (3.28)$$

3.4.1 Column Description

The distillation column considered in this example consists of 5 trays (7 equilibrium stages) with a total condenser and a partial reboiler. The column was assumed to have a constant holdup of 50 kmol on each stage and a constant pressure of 2070 kPa. External heat loss was assumed to be negligible, and the reboiler heat input was set to a constant value. Although a value of the reboiler heat input was not given by Holland and Liapis(12), it was found that use of a value of 15.0 kW at the initial steady state and a value of 22.12 kW after the prescribed feed

disturbance would yield steady state values of column variables that were in close agreement with the reported values.

The feed contains three hydrocarbon components at the mixture boiling point. A complete listing of the feed properties can be found in Table 3.1. Tables 3.2 and 3.3 are comparisons of the initial steady state temperatures and compositions given by Holland and Liapis(12) and the initial steady state values generated in this simulation using the same equilibrium and thermodynamics data.

The disturbance introduced to the column was a feed composition change under the condition that the mixture entered at its boiling point. As can be seen from the feed properties given in Table 3.4, this imposed condition drastically changed the feed temperature.

3.4.2 Simulation Results

Figures 3.1 to 3.4 show the simulated response of the column to the prescribed feed upset using the ASIRK method as compared to that of Holland's θ method. The agreement between the two methods in both the steady state and the transient phase was very close.

To compare the ASIRK method against the constant parameter method of BBSIRK mentioned earlier, the latter method was used to simulate the column again. In these simulations, both methods used the same step size control scheme as proposed by Ballard et al(11). The simulations

Table 3.1

Initial Feed Conditions for Simple Distillation Column

Component number	Name	Flow rate (kmol/s)	Mole fraction
1	C_3H_8	1.000	.600
2	$n-C_4H_{10}$	0.333	.200
3	$n-C_6H_{14}$	0.333	.200

Feed rate = 1.666 kmol/s

Feed temperature = 355 K

Feed pressure = 2070 kPa

Feed stage = 5th

Table 3.2

Comparison of Initial Temperature Profile

Stage	T(K)†	T(K)‡
1	332.0	332.2
2	334.3	334.4
3	337.8	338.0
4	343.3	343.6
5	355.0	355.2
6	366.4	366.6
7	393.5	393.7

Table 3.3

Comparison of Initial Product Compositions

Top	x†	x‡
C_3H_8	.9674	.9677
$n-C_4H_{10}$	.0326	.0323
$n-C_6H_{14}$	.0000	.0000
Bottoms	x†	x‡
C_3H_8	.2326	.2322
$n-C_4H_{10}$	.3674	.3677
$n-C_6H_{14}$	.4000	.4001

† - θ method

‡ - ASIRK method

Table 3.4

Final Feed Conditions of Simple Distillation Problem

Component number	Name	Flow rate (mol/s)	Mole fraction
1	C_3H_8	0.167	.100
2	n- C_4H_{10}	0.667	.400
3	n- C_6H_{14}	0.833	.500

Feed rate = 1.667 mole/s

Feed temperature = 416 K

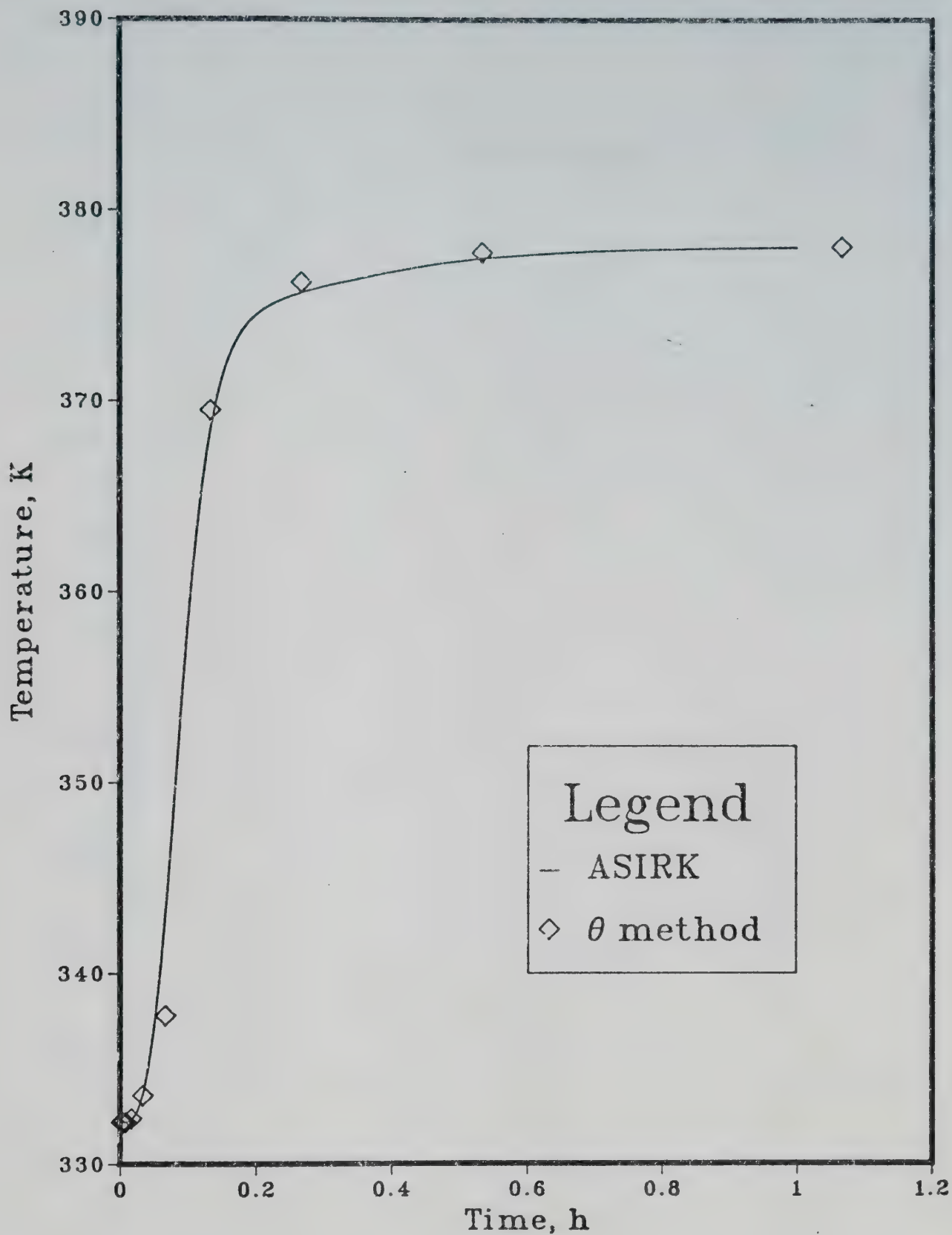


Fig. 3.1 Response of Condenser Temperature to Feed Composition Change

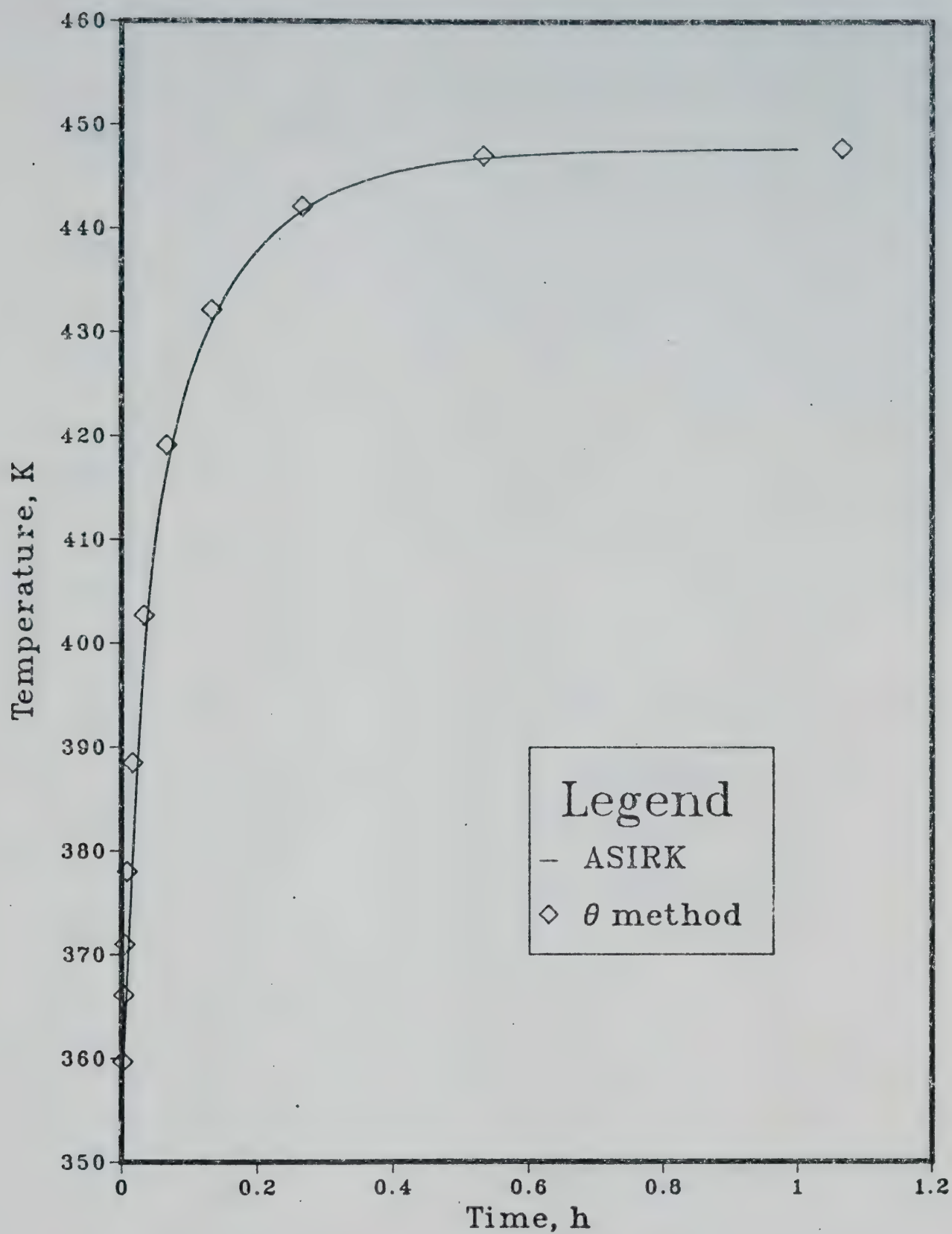


Fig. 3.2 Response of Feed Stage Temperature to Feed Composition Change

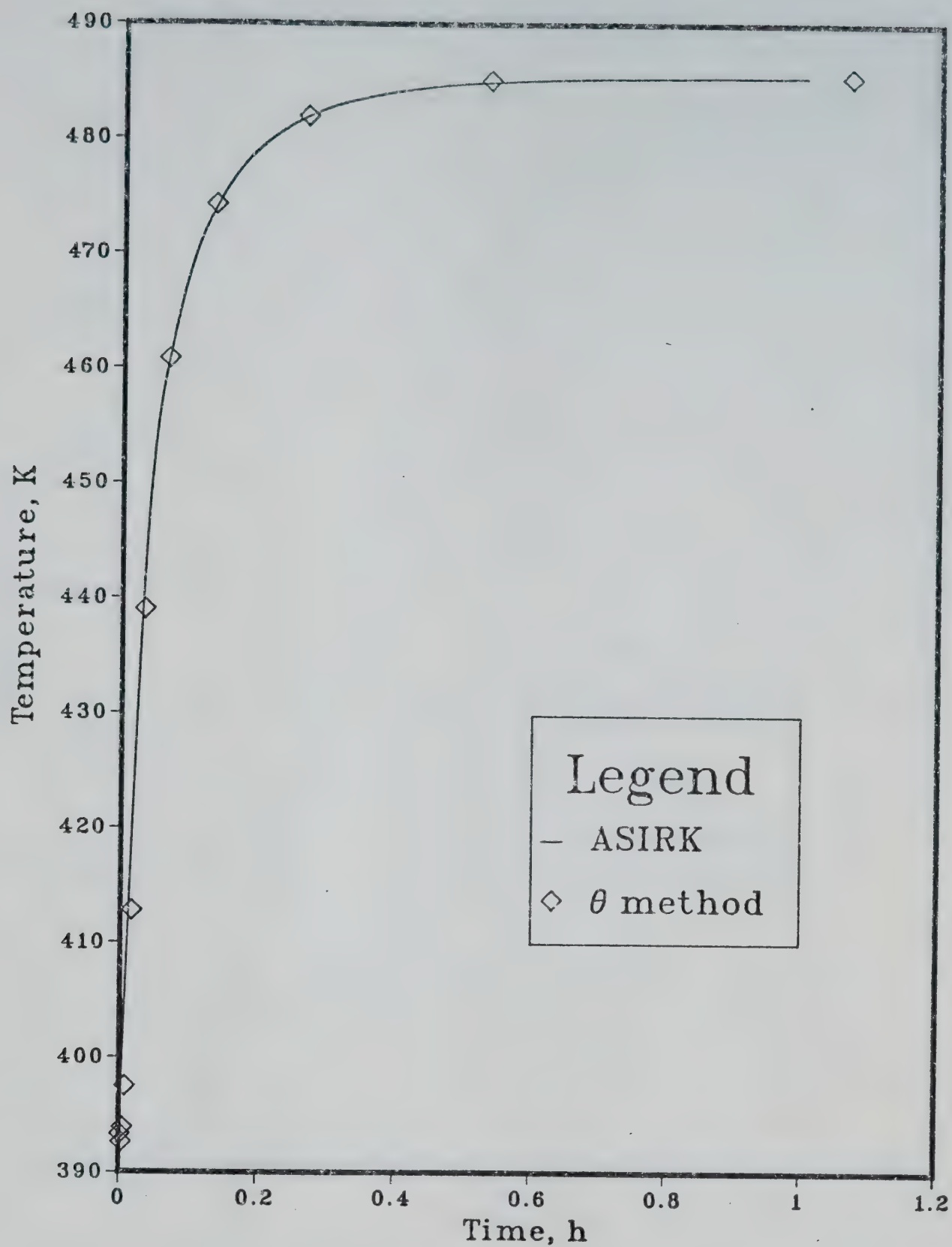


Fig. 3.3 Response of Reboiler Temperature to Feed Composition Change

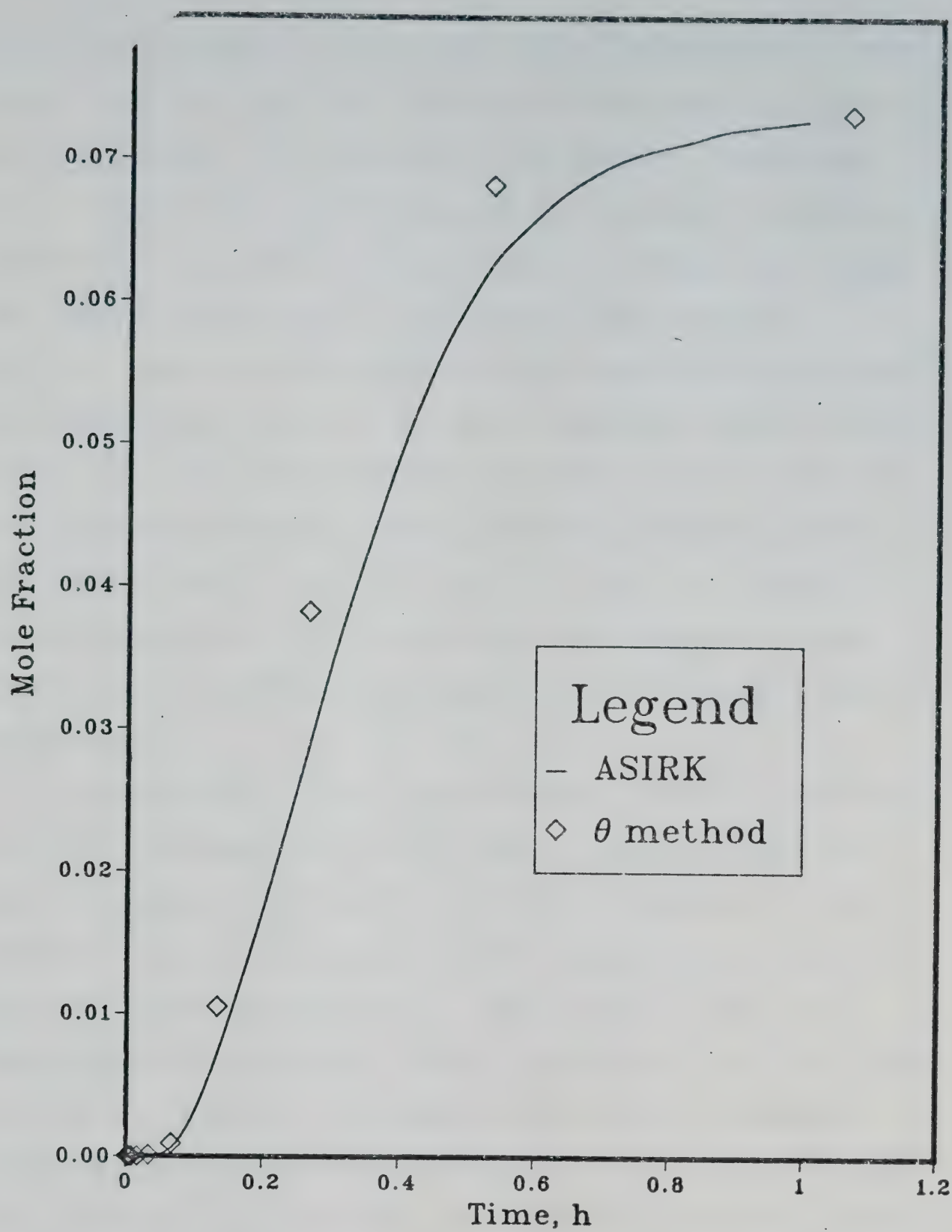


Fig. 3.4 Response of n-C₆ Composition in Condenser

used various values of the error control parameter, σ , that varied from 0.02 to 0.001. The simulation time for each run was 6000 seconds with a maximum time step of 120 seconds.

In Table 3.5, the two methods are compared in terms of computation time and the total number of integration steps. The computation was done on an Amdahl 5860 computer. Table 3.5 shows that the ASIRK method consistently required more computation time for the same simulation partly because of the more complex algorithm. The ASIRK method also took more integration steps than the constant parameter method did. The probable reason for this is that the truncation error estimates of the ASIRK method were generally higher than those of the BBSIRK although no effort has been made to verify this.

The efficiency of the ASIRK method, however, cannot be evaluated by computation time alone. Figure 3.5 and 3.6 show the composition response of the C_6 component in the condenser calculated with the ASIRK method and the constant parameter method respectively. Each figure shows the computed solution at error control parameters of 0.02, 0.005 and 0.001. In Figure 3.5, the solution from the ASIRK method seems to have converged at $\sigma \leq 0.005$. On the other hand, in Figure 3.6, the solution obtained from the constant parameter method still showed an observable change from $\sigma = 0.005$ to $\sigma = 0.001$. In fact, as shown in Figure 3.7, the ASIRK solution at $\sigma = 0.005$ is already comparable to the non-adaptive solution at $\sigma = 0.001$. Relating this

Table 3.5

Comparison of Computation Times for ASIRK and BBSIRK
Solution Methods for Different Values of the Error Control
Parameters

σ	ASIRK		BBSIRK	
	CPU time,s	Number of time steps	CPU time,s	Number of time steps
0.02	0.767	120	0.630	101
0.01	0.966	159	0.719	135
.005	1.151	216	0.926	187
.002	1.616	328	1.301	299
.001	2.115	452	1.722	433

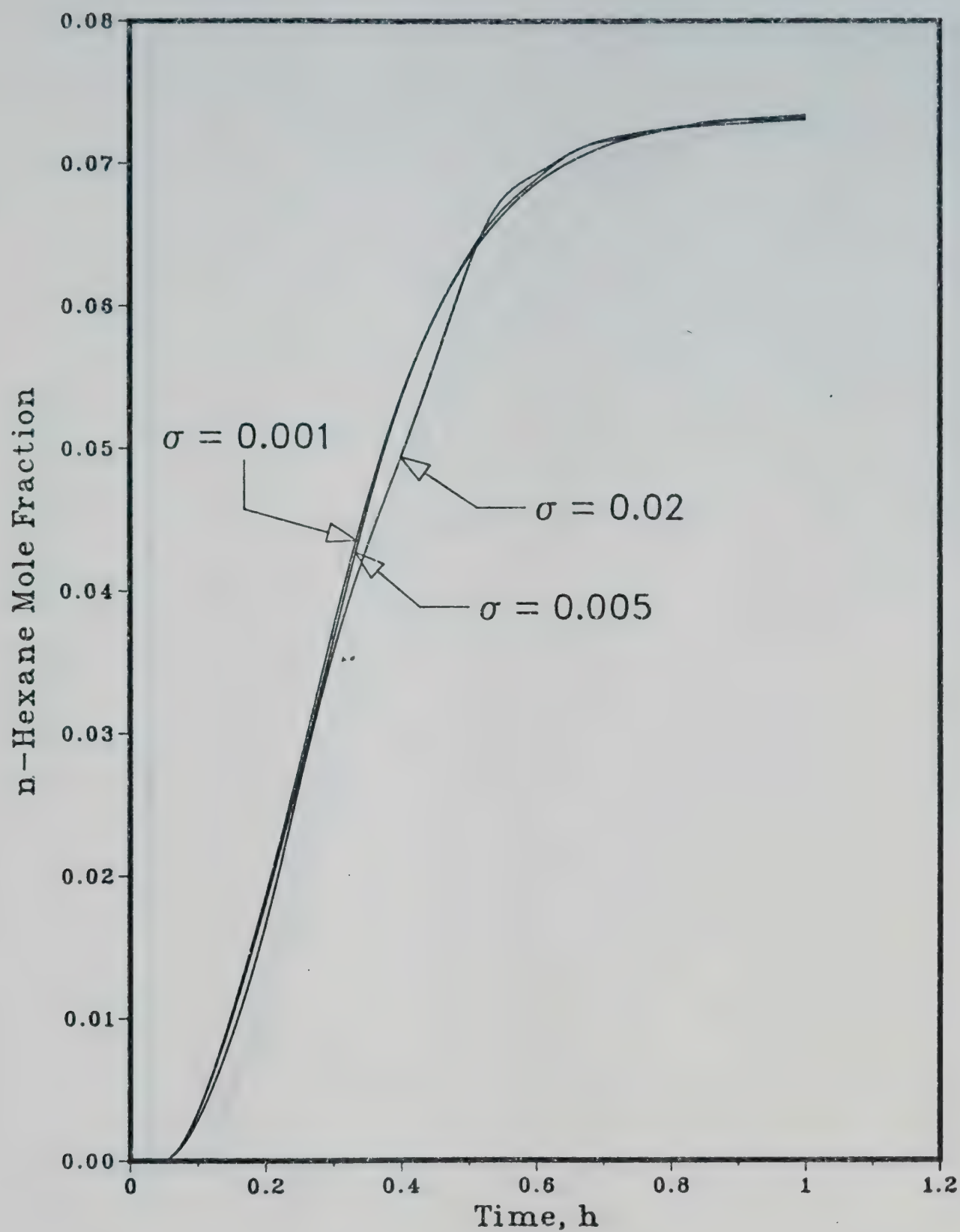


Fig. 3.5 Response of n-C₆ Composition in Condenser Using ASIRK Method

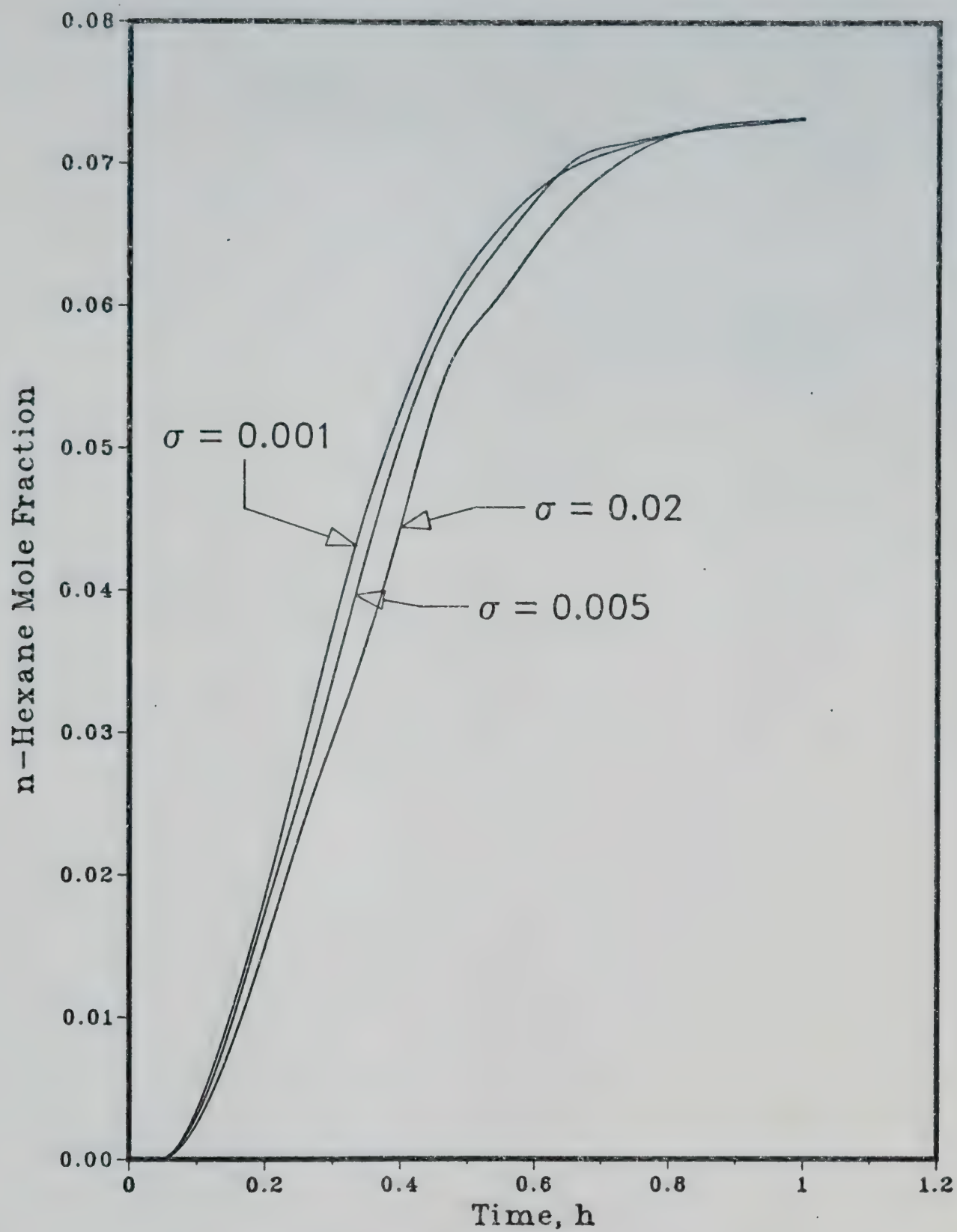


Fig. 3.6 Response of n-C₆ Composition in Condenser Using BBSIRK Method

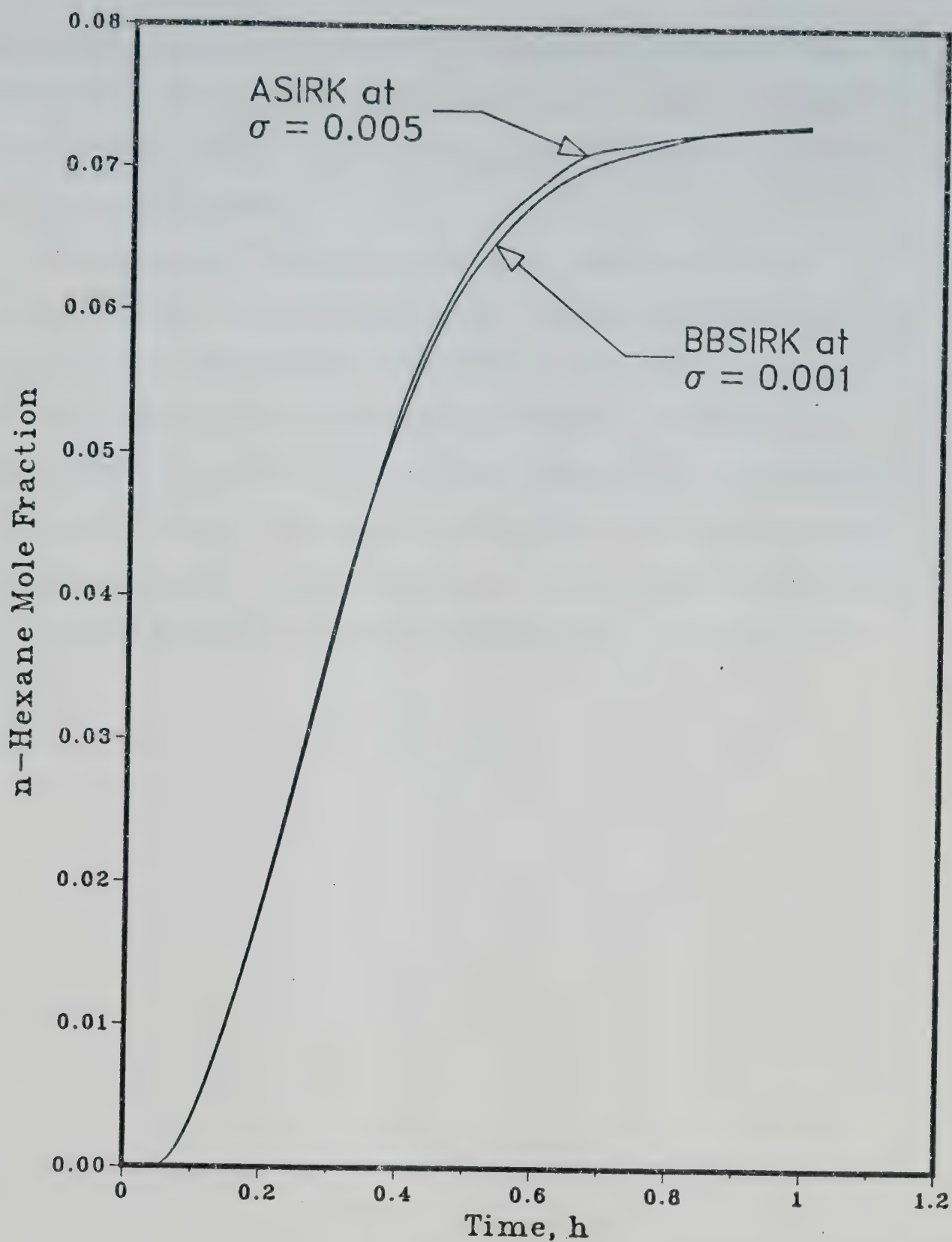


Fig. 3.7 Comparison of the Response of n-C₆ composition in the Condenser Using the ASIRK Method and the BBSIRK Method

performance to the information in Table 3.5 reveals that the ASIRK method can produce approximately the same accuracy in 1.151 seconds of CPU time as the constant parameter method can in 1.722 seconds.

The numerical example presented above is not an extensive study of the performance of the ASIRK method, and it is quite possible that some other SIRK methods can be even more efficient than the ASIRK method. However the ASIRK method has nevertheless been shown to be a competitive integration algorithm through the study of Prokopakis(19) and this example. Based on these results, the ASIRK method was adopted for all subsequent simulations in this study.

4. Simulation of a Hydrocarbon Separator

In simulating the behavior of a multicomponent industrial column, Stathaki et al(26) found the response of the column to certain disturbances to exhibit some very interesting characteristics.

One of the characteristics is inverse response, where the direction of change of a variable switches from one to the other during the transient period and crosses over the initial steady state value before reaching a final steady state. The variables found to exhibit inverse behavior were compositions only, as Stathaki et al stated

... no inverse responses were observed for the tray temperatures nor for the key components when they were present as impurities, ie. the light key in the bottoms and the heavy key in the distillate.

Another characteristic is asymmetric dynamics of the column. At some operating conditions, the time required for the column to change between two steady states can differ significantly depending on the direction of change. For example, Stathaki and co-workers reported

... the transition from Steady State 1 to Steady State 2 has response times as large as 1000 minutes ... The reverse transition (2→1) has response times which are all less than 220 minutes.

Such nonlinear column dynamic behavior, if not handled properly, can lead to unsatisfactory control performance. Therefore it is of great interest to establish if these characteristics are common to the distillation process in general, and to investigate the causes of these phenomena. In the example considered in this chapter, the dynamic simulator is used to obtain the transient response of a distillation column subject to disturbances so that the results will lead to an explanation for the inverse dynamic behavior of distillation column.

4.1 Description of the Hydrocarbon Separator

The hydrocarbon separator used for this example has been simulated by Cook(30) to demonstrate use of a dynamic simulator developed at Case Western Reserve University. However the dynamic behavior of the column was not discussed and the type of disturbance introduced to the column was limited to a change of feed composition only. The simulation performed in this work employed different process parameters and operating conditions than those used by Cook.

The column has 29 plates so including the partial condenser and the reboiler a total of 31 stages. The feed mixture contains five light hydrocarbon components and is fed to the column at the 12th plate. Table 4.1 is a list of column specifications that are pertinent to the simulation. The column is assumed to have a constant molar holdup for all stages, and that all tray efficiencies are 100%.

Table 4.1
Hydrocarbon Column Specifications

No. of Stages	31
No. of Components	5
No. of Feeds	1
Feed Plate Number	12
Column Pressure	101.3 kPa
Tray Holdup	14.0 kmol
Reboiler Holdup	50.0 kmol
Condenser Holdup	50.0 kmol
Reflux Rate	1.5 kmol/s
Tray Efficiency	100 %

Furthermore, the reflux rate is held constant except for tests involving reflux changes, and the heat loss to the environment is assumed negligible.

The simulations are performed for three different types of disturbances which are common to industrial columns.

These disturbances are

- i. changes in feed flow rate;
- ii. changes in reboiler heat input;
- iii. changes in reflux rate.

In all of these simulations, each disturbance is introduced individually to the column so that the net effect of the particular disturbance is more observable. Table 4.2 provides a summary of the initial feed properties, and Table 4.3 is a partial listing of the initial steady state values of the variables.

Table 4.2
Feed Specifications

Initial Feed Rate		0.8333 kmol/s
Feed Temperature		353.0 K
Feed Pressure		101.3 kPa
<u>Compositions (mole %):</u>		
1	Ethane	3.0
2	Propylene	40.0
3	Propane	15.0
4	Iso-butane	15.0
5	Cis-butene-2	27.0

Table 4.3

Selected Initial Conditions of Hydrocarbon Separator

Stage	Temp. (K)	Compositions				
		x_1	x_2	x_3	x_4	x_5
1	328.88	0.0264	0.6755	0.2654	0.0304	0.0022
5	335.33	0.0103	0.5624	0.2706	0.1302	0.0265
10	346.42	0.0101	0.4173	0.1931	0.2234	0.1561
13	352.64	0.0097	0.3599	0.1587	0.1963	0.2754
15	355.20	0.0027	0.3319	0.1647	0.2109	0.2897
20	362.68	0.0001	0.2309	0.1542	0.2681	0.3466
25	373.13	0.0000	0.1195	0.1053	0.3424	0.4328
31	386.47	0.0000	0.0240	0.0287	0.3248	0.6225

Stage	Liquid rate (kmol/s)	Vapor rate (kmol/s)
1	1.500	0.474
5	1.222	1.770
10	1.012	1.499
13	1.521	1.488
15	1.490	1.146
20	1.370	1.037
25	1.241	0.902
31	0.361	0.862

Condenser load = 7.883 kW

Reboiler load = 8.333 kW

Reflux ratio = 3.1729

4.1.1 Simulation Results for Feed Rate Changes

Feed rate disturbances of varying magnitude, as shown in Table 4.4, are introduced to the column. The maximum change is restricted to within $\pm 30\%$ around the initial value of 0.8333 kmol/s.

Figure 4.1 is a plot of the steady state temperature profiles for feed changes. The feed disturbances have much greater effect on the temperatures in the stripping section of the column than on the temperatures in the enriching section. Figures 4.2 and 4.3 show the steady state composition profiles of the light key component (iso-butane) and the heavy key component (cis-butene-2).

The dynamic response of the column to feed rate changes exhibits inverse behavior in the composition response of the key components in the product streams. For all of the tests performed, the light key composition in the distillate and the heavy key composition in the bottoms product have inverse behavior as shown in Figures 4.4 and 4.5 respectively. These responses exhibit similar behavior to that reported by Stathaki and co-workers(26). However, for this column the occurrence of inverse response is not limited to key components in the product streams, as inverse behavior can also be found in other trays with other components.

It was also discovered that even some of the stage temperatures exhibit inverse behavior, especially in the enriching section. Ironically, as pointed out before, the

Table 4.4
Simulations for Feed Flow Rate Changes

Test No.	Change	New Feed Rate (kmol/s)
CK.FD.OL11	+ 5%	0.8750
CK.FD.OL12	- 5%	0.7917
CK.FD.OL13	+10%	0.9167
CK.FD.OL14	-10%	0.7500
CK.FD.OL15	+20%	1.0000
CK.FD.OL16	-20%	0.6667
CK.FD.OL17	+30%	1.0833
CK.FD.OL18	-30%	0.5833

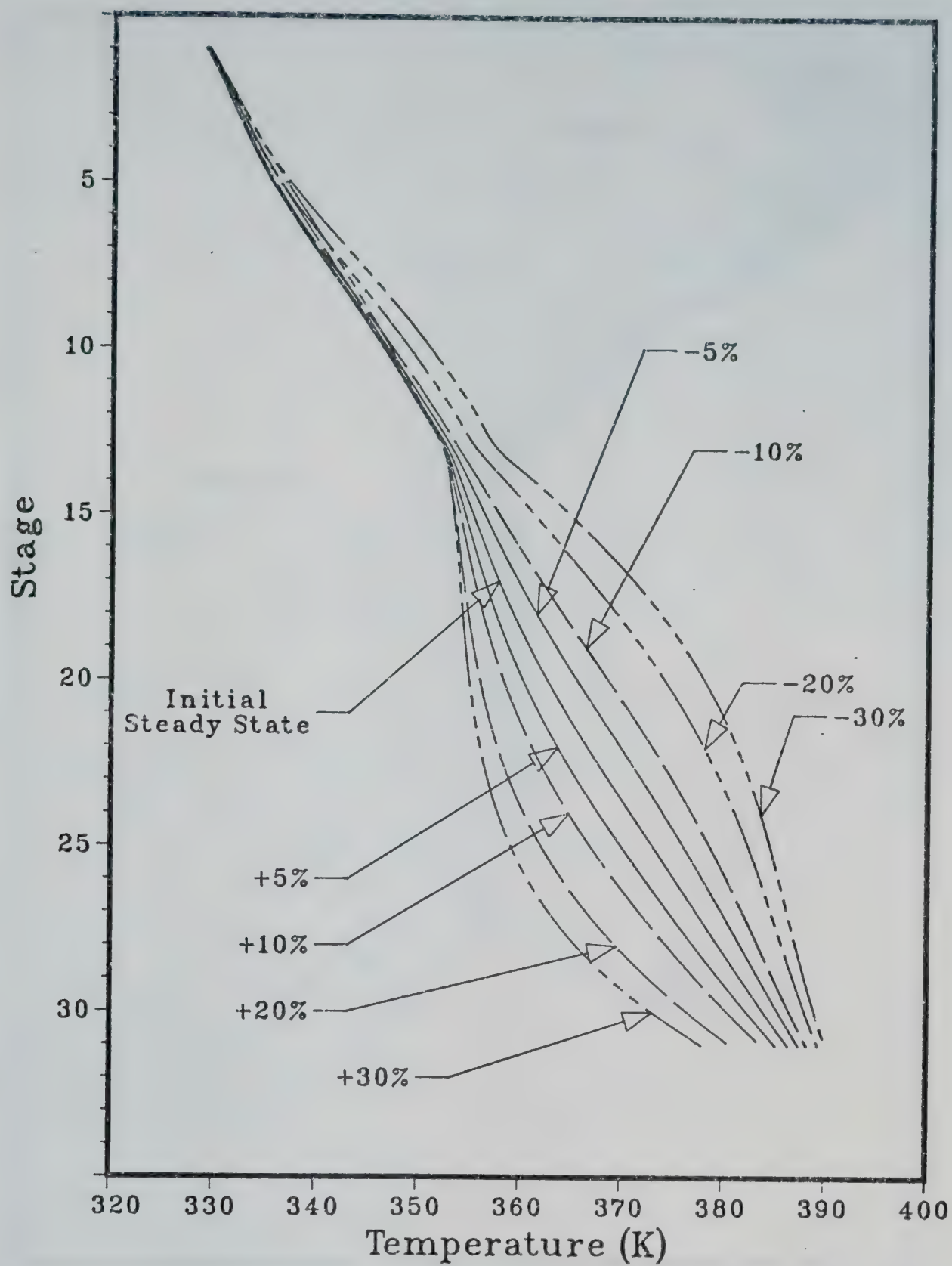


Fig. 4.1 Steady State Temperature Profiles for Feed Flow Rate Changes

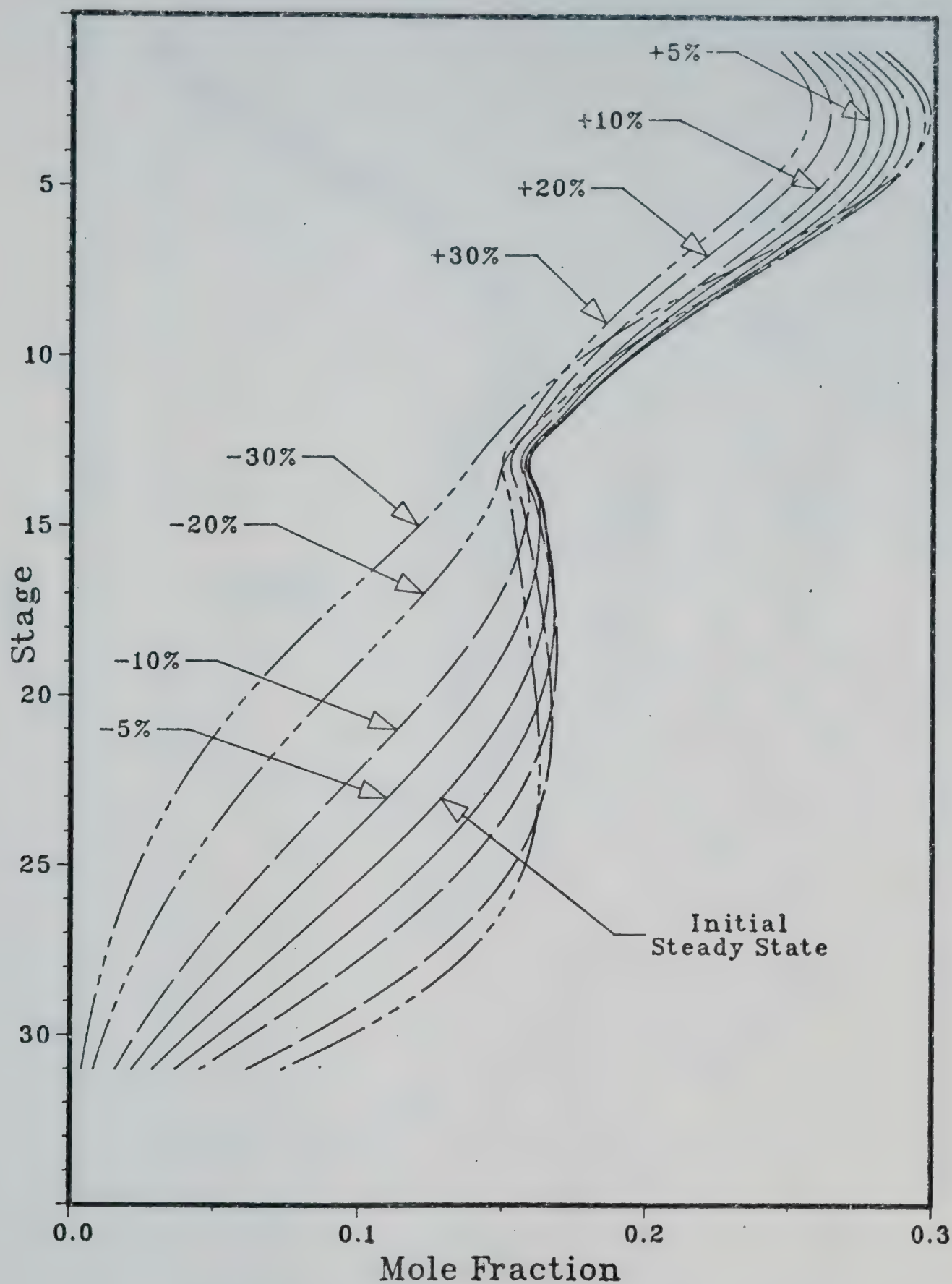


Fig. 4.2 Steady State Light Key Composition Profiles for Feed Flow Rate Changes

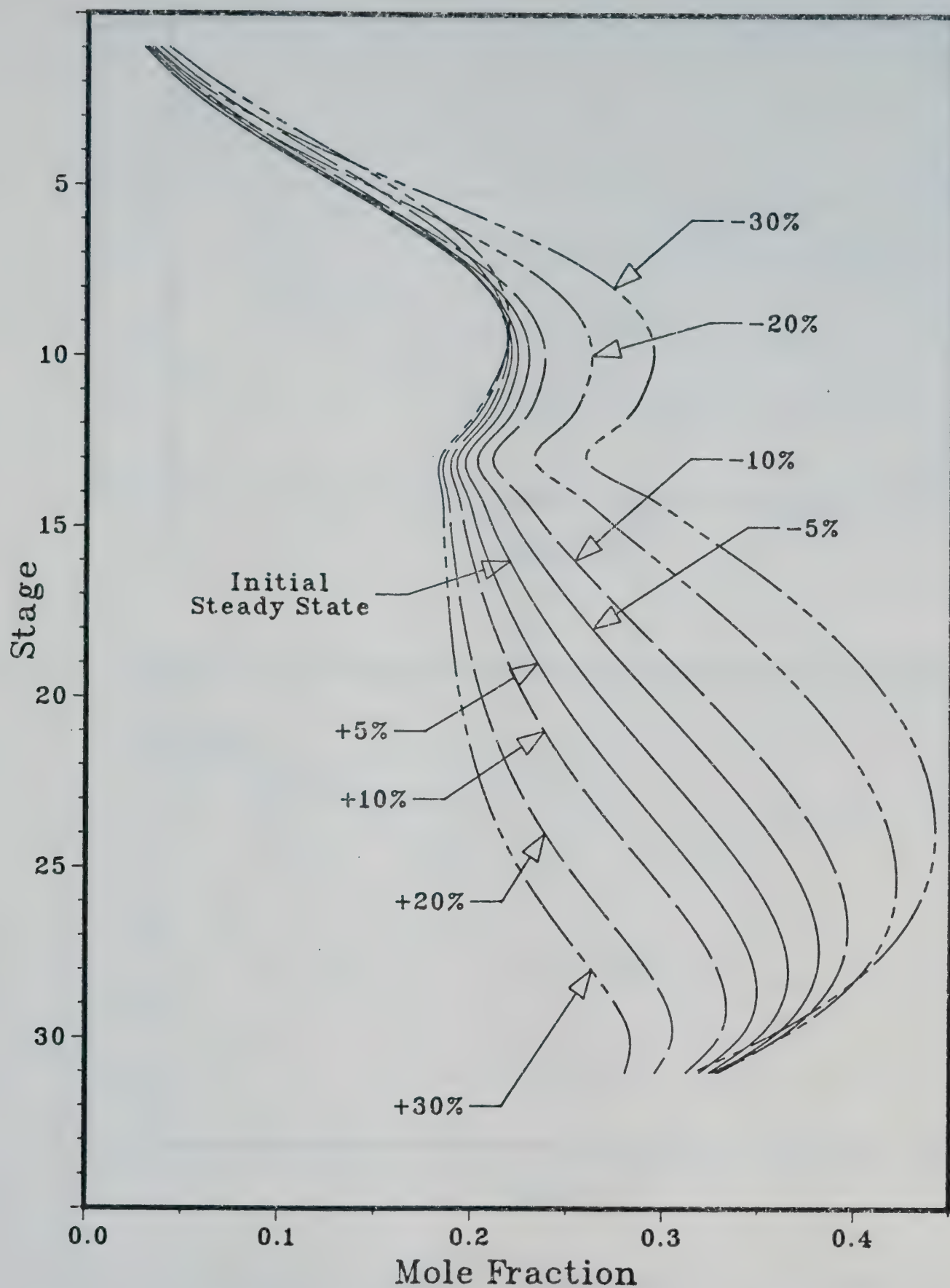


Fig. 4.3 Steady State Heavy Key Composition Profiles for Feed Flow Rate Changes

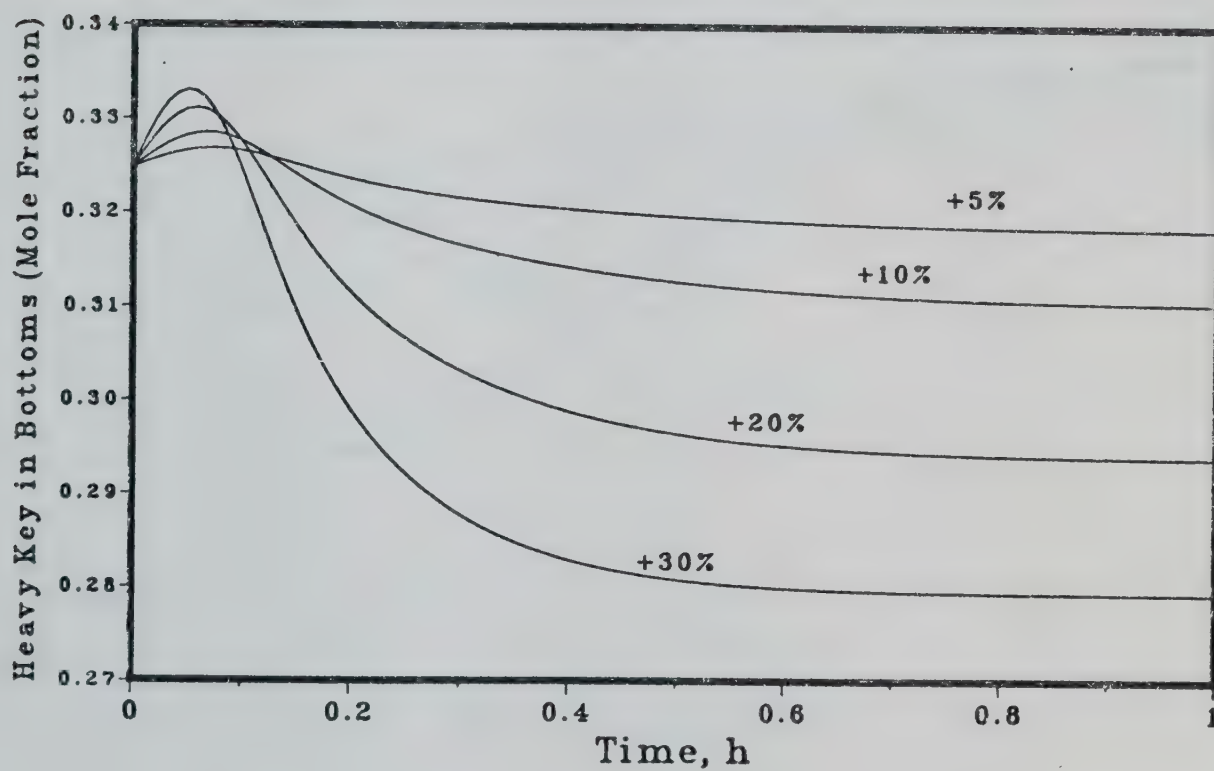
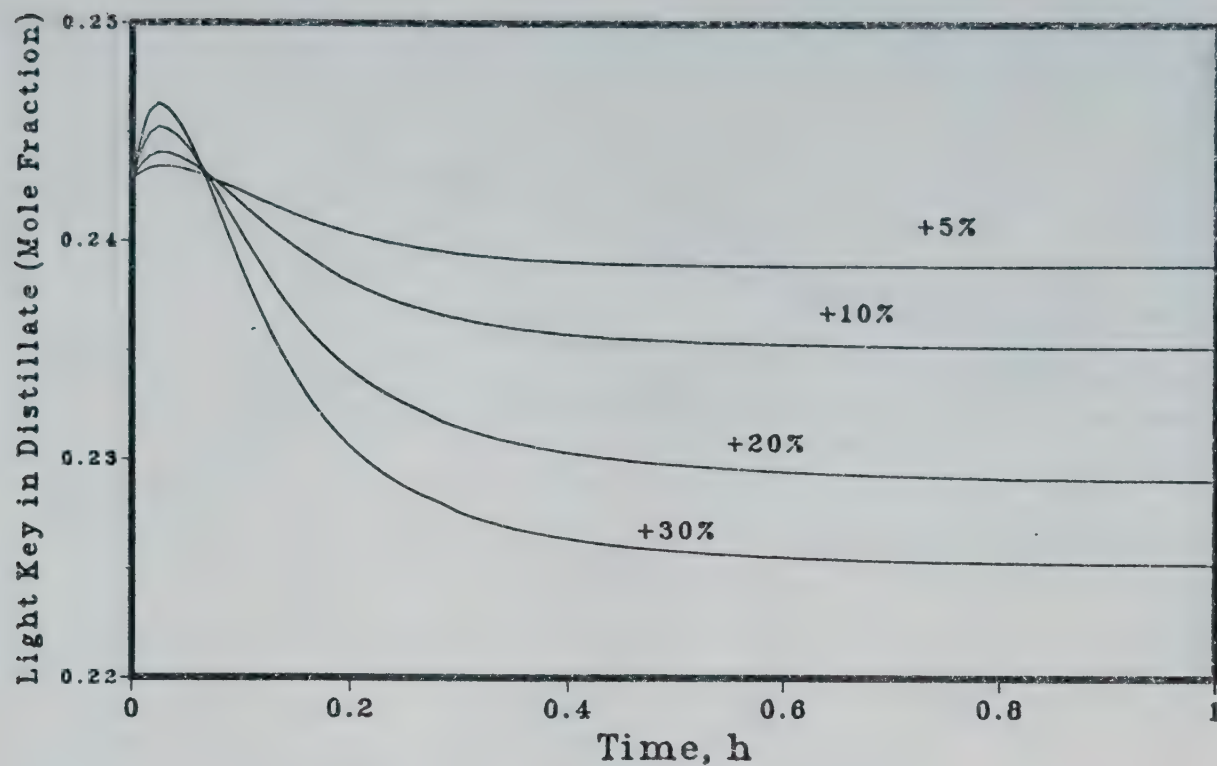


Fig. 4.4 Response of Product Compositions to Increases in Feed Flow Rate

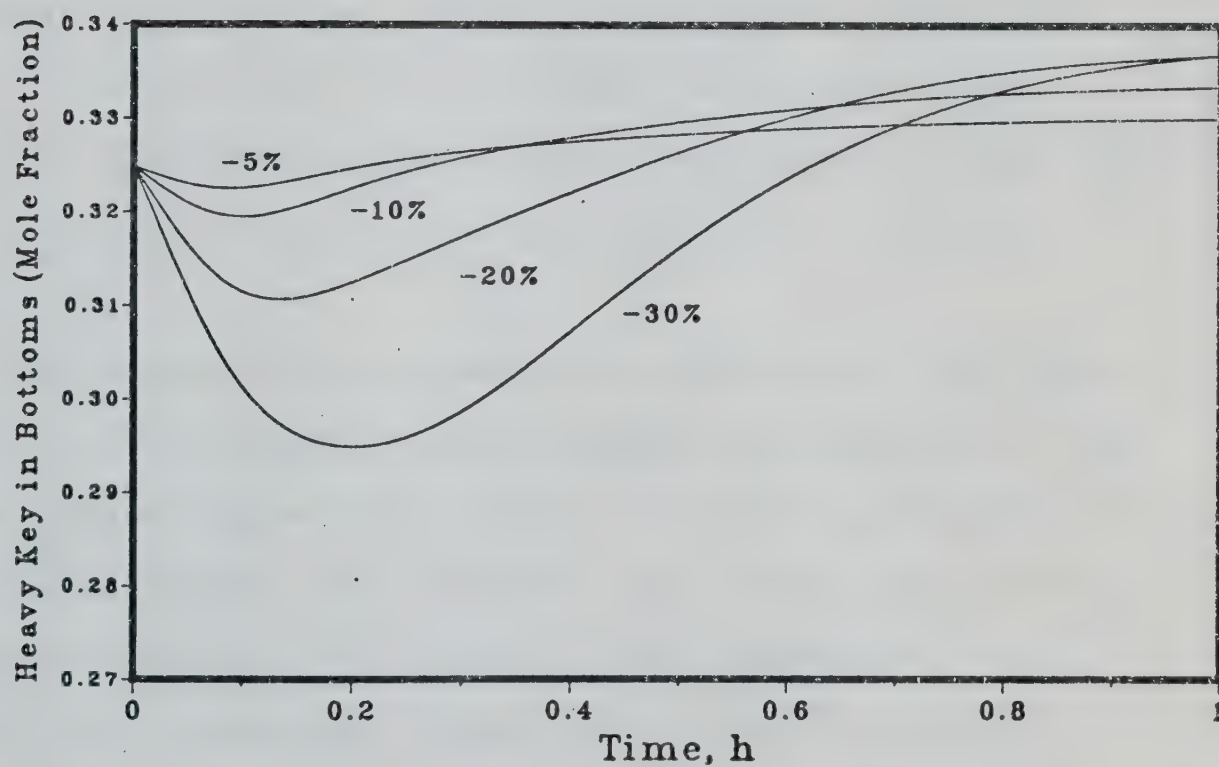
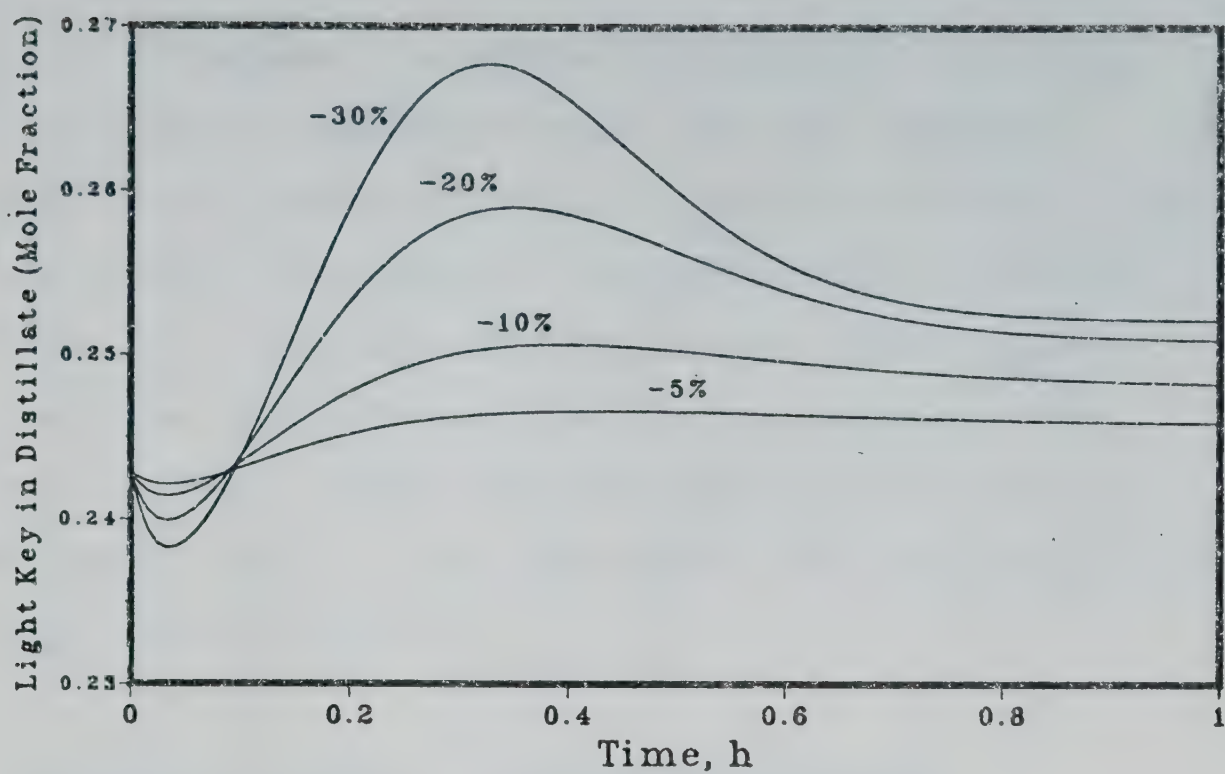


Fig. 4.5 Response of Product Compositions to Decreases in Feed Flow Rate

steady state temperatures of the enriching section do not shift very much in response to the feed rate changes compared to the temperatures in the stripping section. The inverse behavior is especially pronounced with a decrease in feed rate, in which case the temperature of all stages at and above the feed location show inverse response. The transient values of some selected stage temperatures are summarized in Table 4.5 for the case of $\pm 10\%$ feed changes to show the inverse response.

4.1.2 Simulation Results for Heat Input Changes

Similar to the tests performed for feed rate changes, the heat input to the reboiler is perturbed around the initial steady state value of 8.333 kW to obtain the transient response of the column to changes in boilup rate. The perturbed values of the heat input are listed in Table 4.6.

The steady state temperature profiles for heat input changes to the reboiler are presented in Figure 4.6. The steady state composition profiles for the key components are plotted in Figures 4.7 and 4.8. The results show that an increase in heat input drives up the temperature on all stages, and a decrease in heat input has the opposite effect. The steady state gains for the change in stage temperatures are in general higher for negative than for positive changes in heat input.

Table 4.5
Temperature Response for 10% Feed Rate Change

+10% Feed Rate Change

Time (h)	Temperature, K			
	T_1	T_{10}	T_{20}	T_{31}
0.0	328.880	346.420	362.680	386.470
.0167	328.969	346.600	362.369	386.295
.0333	328.968	346.725	362.103	386.096
.0833	328.956	345.818	361.337	385.545
.1667	328.930	346.662	360.167	384.936
.3333	328.882	346.413	358.823	384.203
.6667	328.863	346.303	358.111	383.738
1.000	328.858	346.293	358.010	383.672

-10% Feed Rate Change

Time (h)	Temperature, K			
	T_1	T_{10}	T_{20}	T_{31}
0.0	328.880	346.420	362.680	386.470
.0167	328.781	346.240	363.005	386.639
.0333	328.774	346.104	363.302	386.824
.0833	328.797	345.995	364.198	387.312
.1667	328.834	346.276	365.761	387.787
.3333	328.917	346.959	367.916	388.177
.6667	328.948	347.305	368.854	388.277
1.000	328.944	347.290	368.848	388.239

Table 4.6

Simulations for Changes in Heat Input Rate

Test No.	Change	New Input Rate (kW)
CK.QR.OL11	+ 5%	8.750
CK.QR.OL12	- 5%	7.917
CK.QR.OL13	+10%	9.167
CK.QR.OL14	-10%	7.500
CK.QR.OL15	+15%	9.583
CK.QR.OL16	-15%	7.083
CK.QR.OL17	+20%	10.00
CK.QR.OL18	-20%	6.667

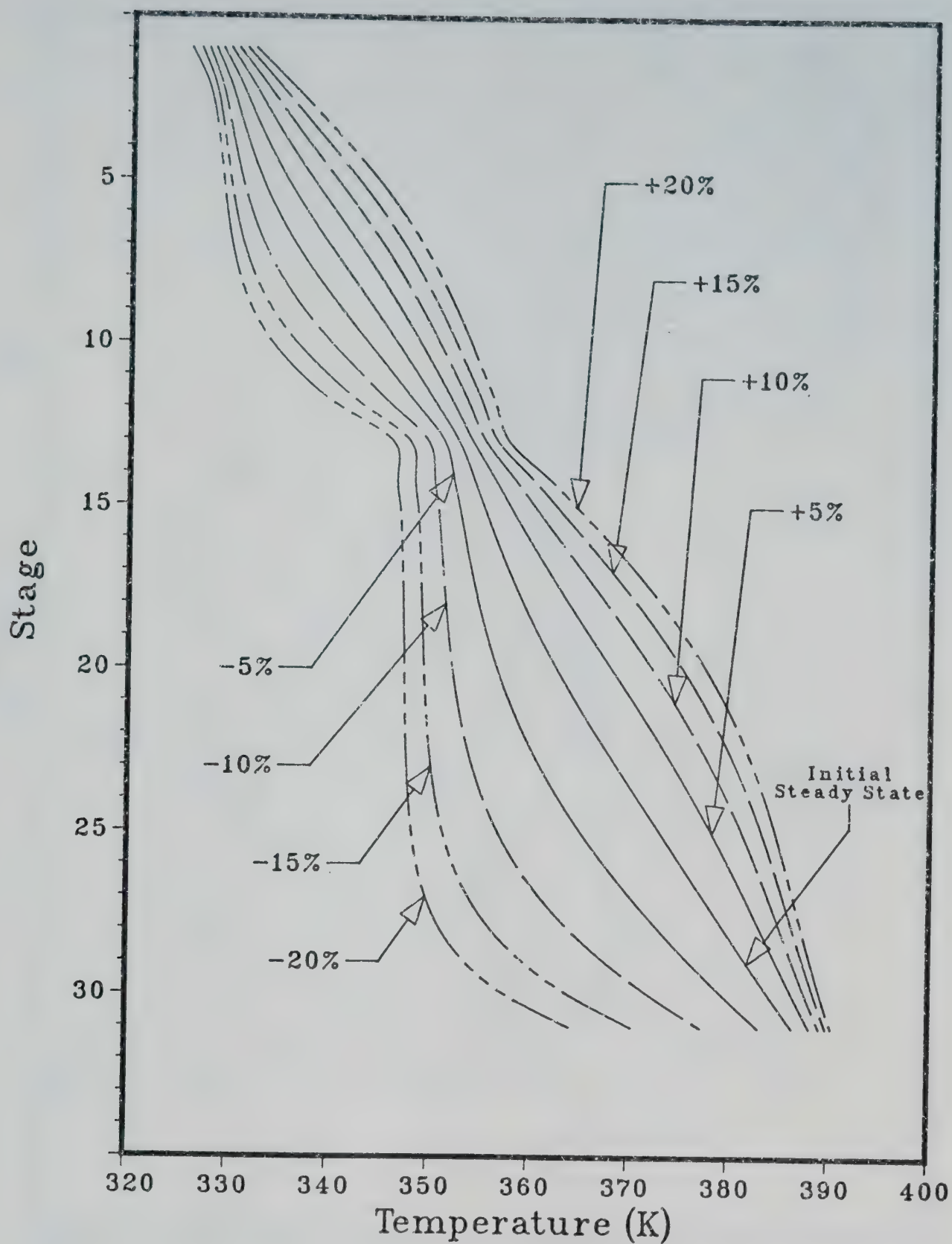


Fig. 4.6 Steady State Temperature Profiles for Heat Input Changes

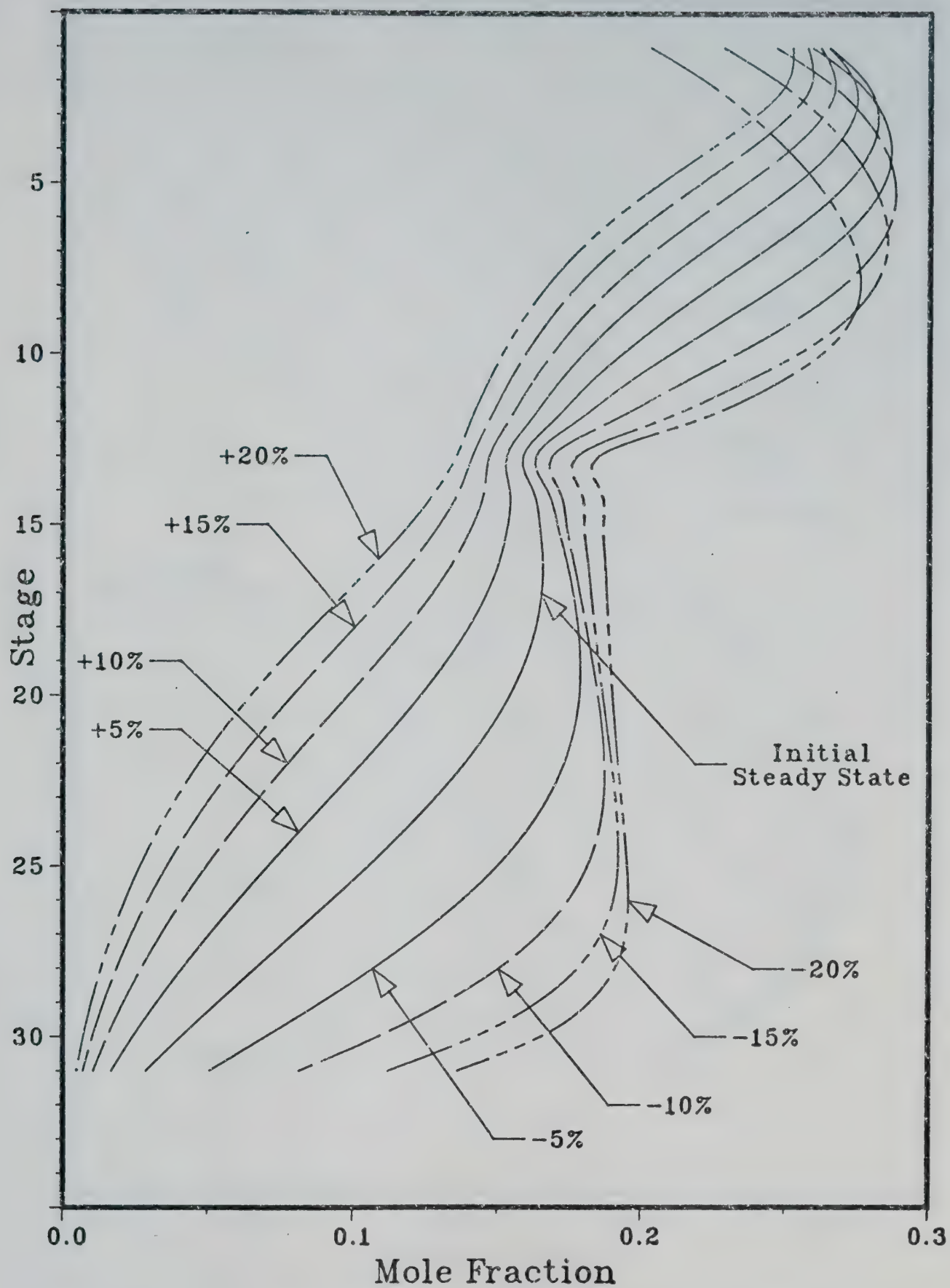


Fig. 4.7 Steady State Light Key Composition Profiles for Heat Input Changes

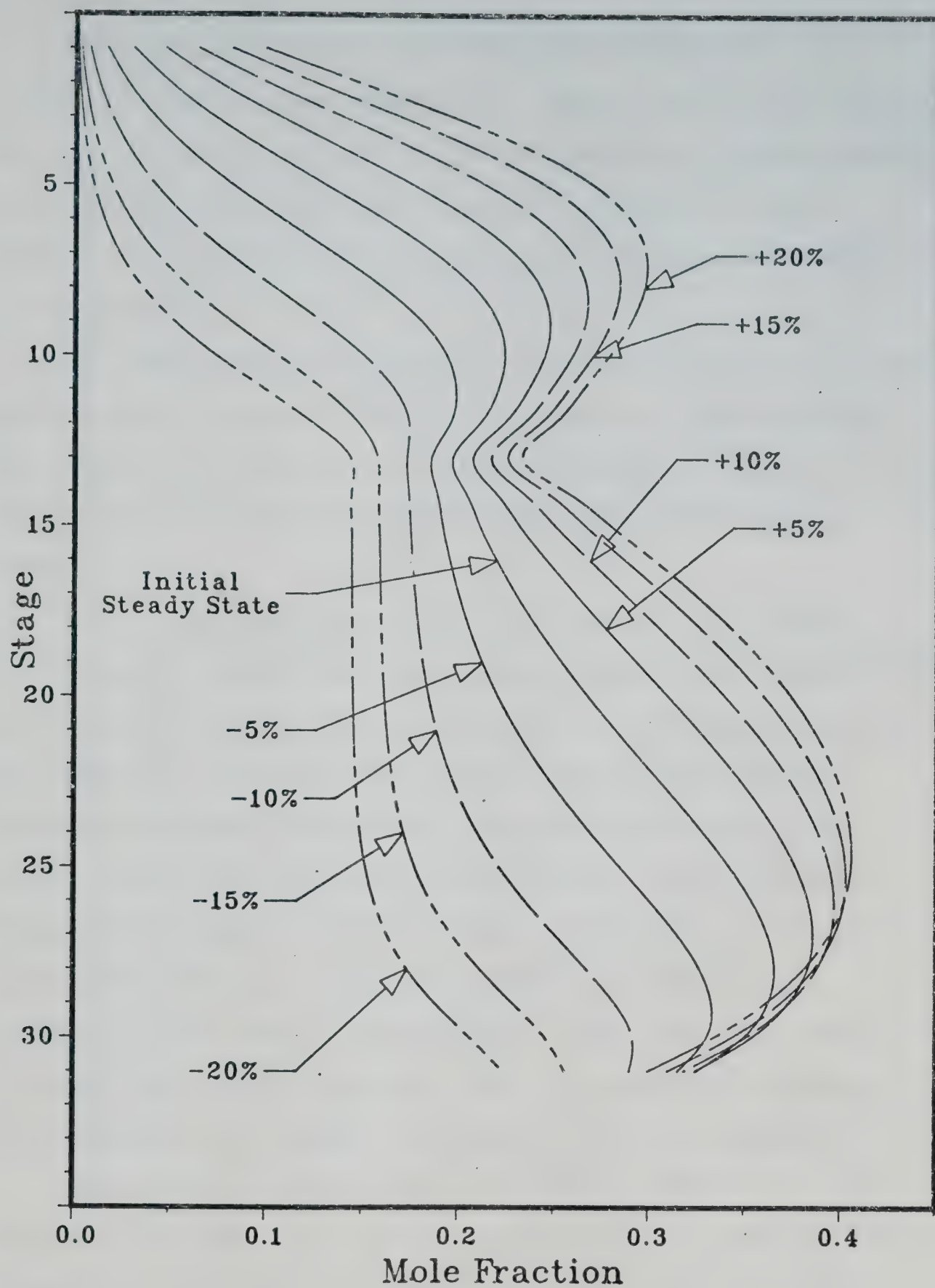


Fig. 4.8 Steady State Heavy Key Composition Profiles for Heat Input Changes

Inverse response is also found in the product composition of the key components. Specifically, the light key (iso-butane) composition in the distillate shows inverse behavior for positive input changes in Figure 4.9 yet exhibits no inverse behavior for negative changes as shown in Figure 4.10.

The heavy key (cis-butene-2) composition in the bottoms product shows inverse behavior for negative input changes. The response to the positive input changes, as shown in Figure 4.9, is also characterized by nonminimum phase behavior.

Luyben(24) concluded from his analysis of a binary distillation column that the inverse response in composition to disturbances in vapor boil-up rate is contributed by the 'K₂ effect'. This term refers to the situation when an increase in vapor flow pushes part of the froth off the trays, producing a hydraulic disturbance. The hydraulic disturbance coupled with the vapor increase may under some conditions produce inverse responses in compositions. However in this model the holdups on the trays are assumed constant and cannot be pushed over to create the hydraulic disturbance, yet inverse response can still be observed.

Unlike the results obtained from the simulation for feed rate changes, no inverse response can be observed for components other than the key components. The number of variables exhibiting inverse response is also significantly less than that for feed rate changes. Furthermore, for

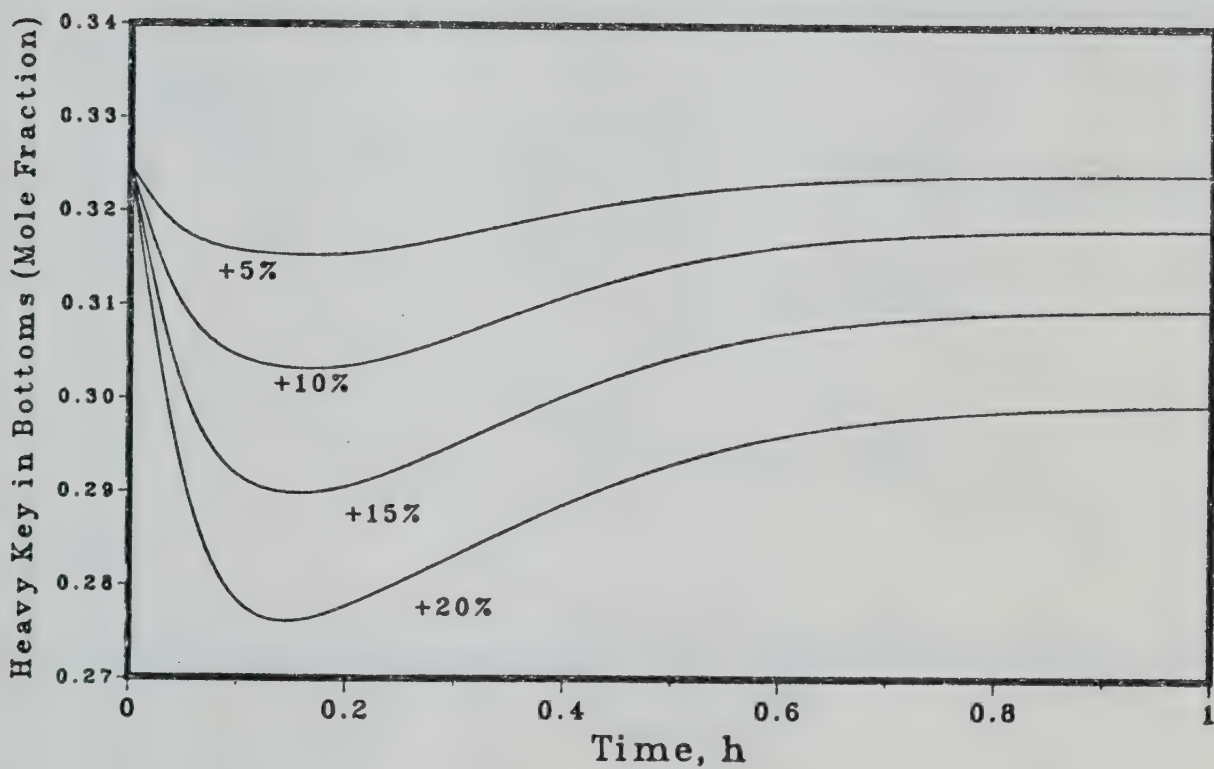
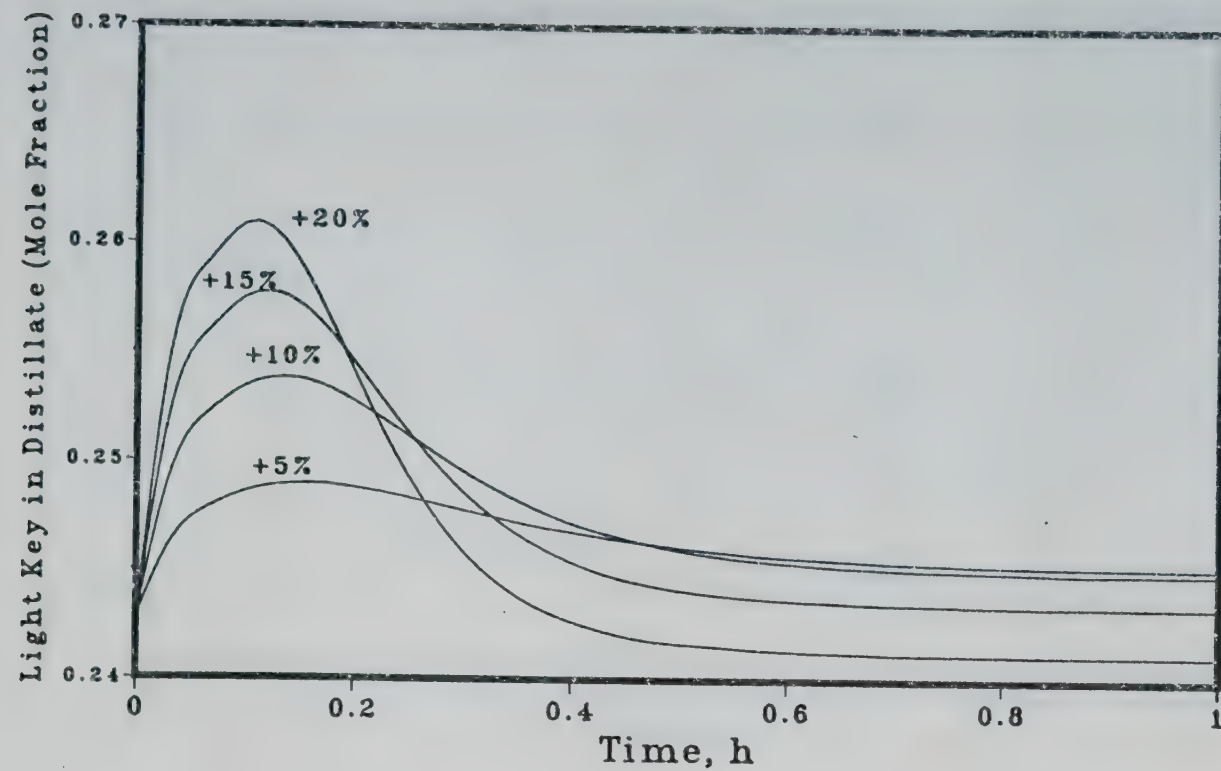


Fig. 4.9 Response of Product Compositions to Increases in Heat Input

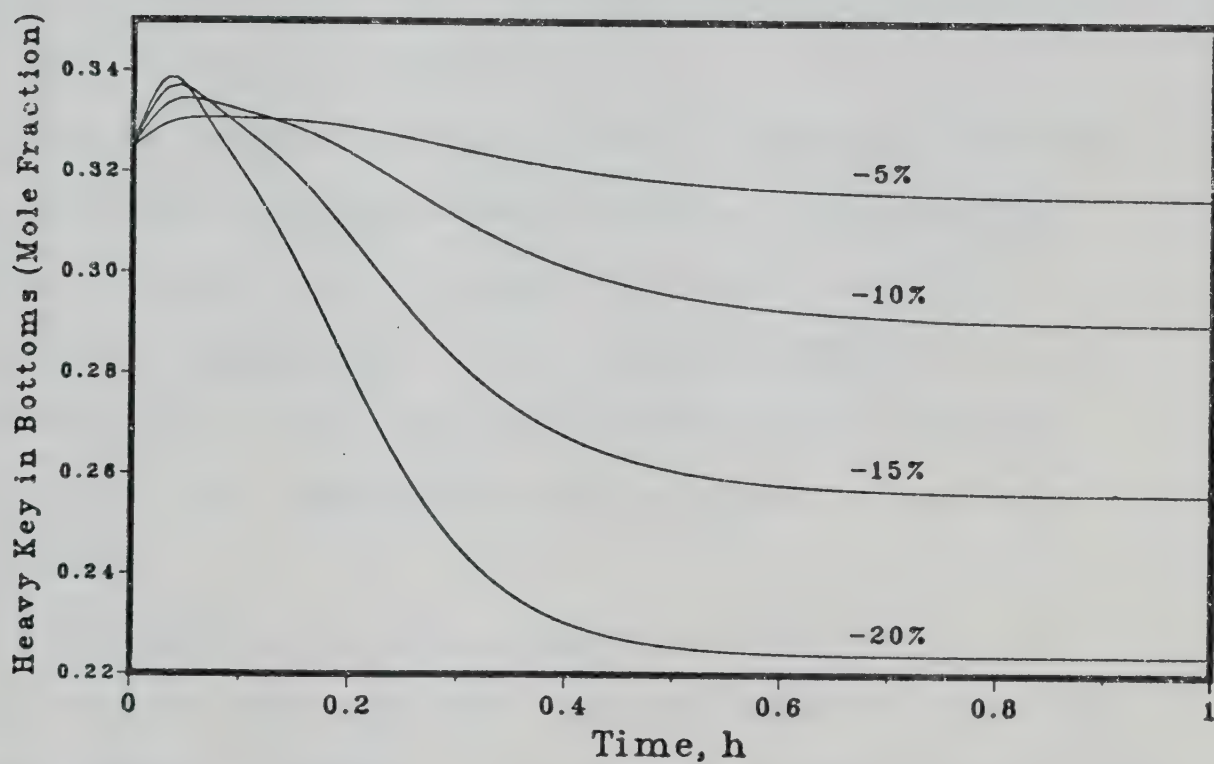
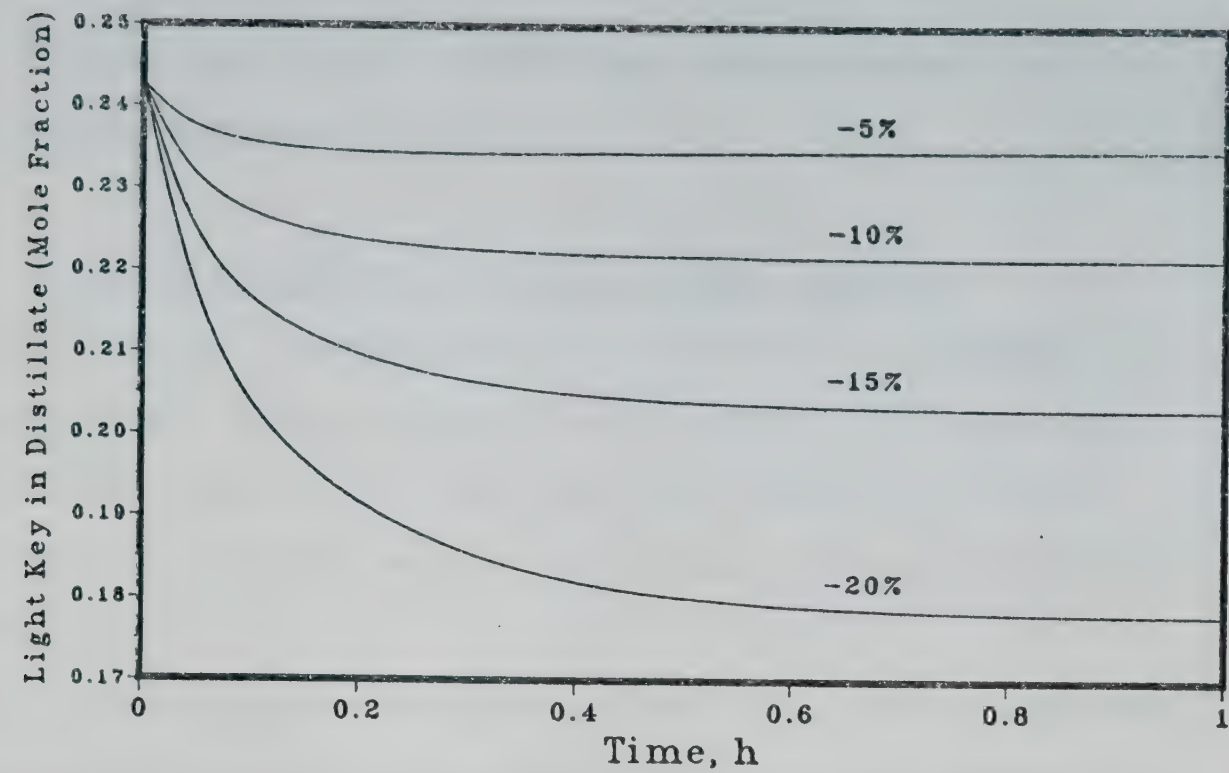


Fig. 4.10 Response of Product Compositions to Decreases in Heat Input

these disturbances none of the stage temperatures exhibited any inverse response behavior.

4.1.3 Simulation Results for Reflux Rate Changes

To simulate the dynamics of the column in response to reflux changes, step changes in the reflux flow rate are made around the initial value of 1.500 kmol/s. The new, final steady state values of the reflux rate, are listed in Table 4.7.

The steady state temperature profiles for the different reflux rates are plotted in Figure 4.11 and the composition profiles of the light heavy key components presented in Figures 4.12 and 4.13 respectively.

Inverse response of the product composition is also observed with this type of disturbance. For positive changes in reflux rate, as shown in Figure 4.14, the cis-butene-2 composition in the bottoms exhibits inverse behavior in all tests, yet no inverse behavior can be observed for the composition of iso-butane in the distillate.

For negative changes as shown in Figure 4.15, the composition of the heavy key component does not show any inverse behavior except in a few stages immediately at and above the feed stage. However, the distillate composition of the light key component does exhibit inverse behavior in all tests.

Table 4.7

Simulations for Changes in Reflux Rate

Test No.	Change	New Rate (kmol/s)
CK.RF.OL11	+ 5%	15.75
CK.RF.OL12	- 5%	14.25
CK.RF.OL13	+10%	16.50
CK.RF.OL14	-10%	13.50
CK.RF.OL15	+20%	18.00
CK.RF.OL16	-20%	12.00
CK.RF.OL17	+25%	18.75
CK.RF.OL18	-25%	11.25

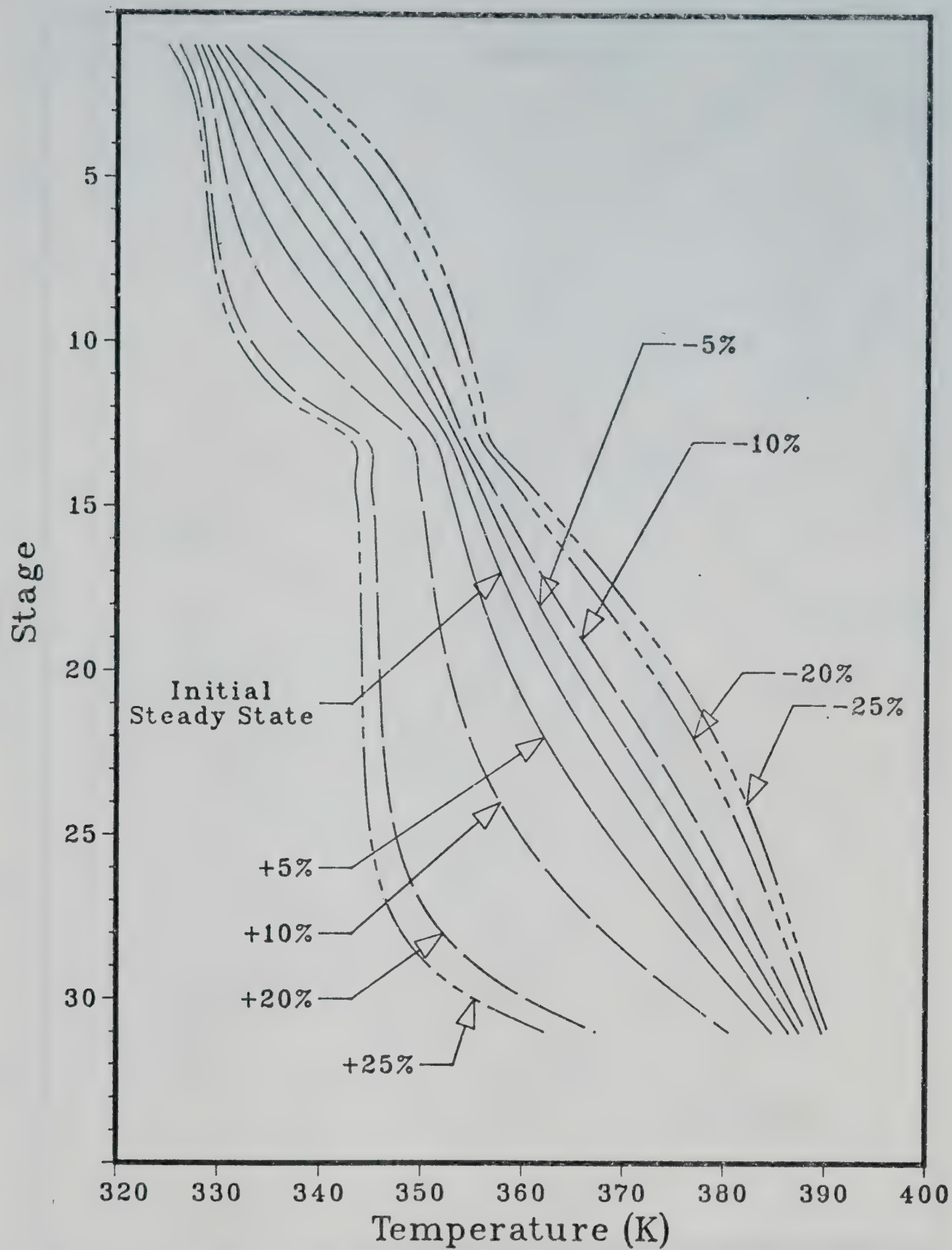


Fig. 4.11 Steady State Temperature Profiles for Reflux Flow Rate Changes

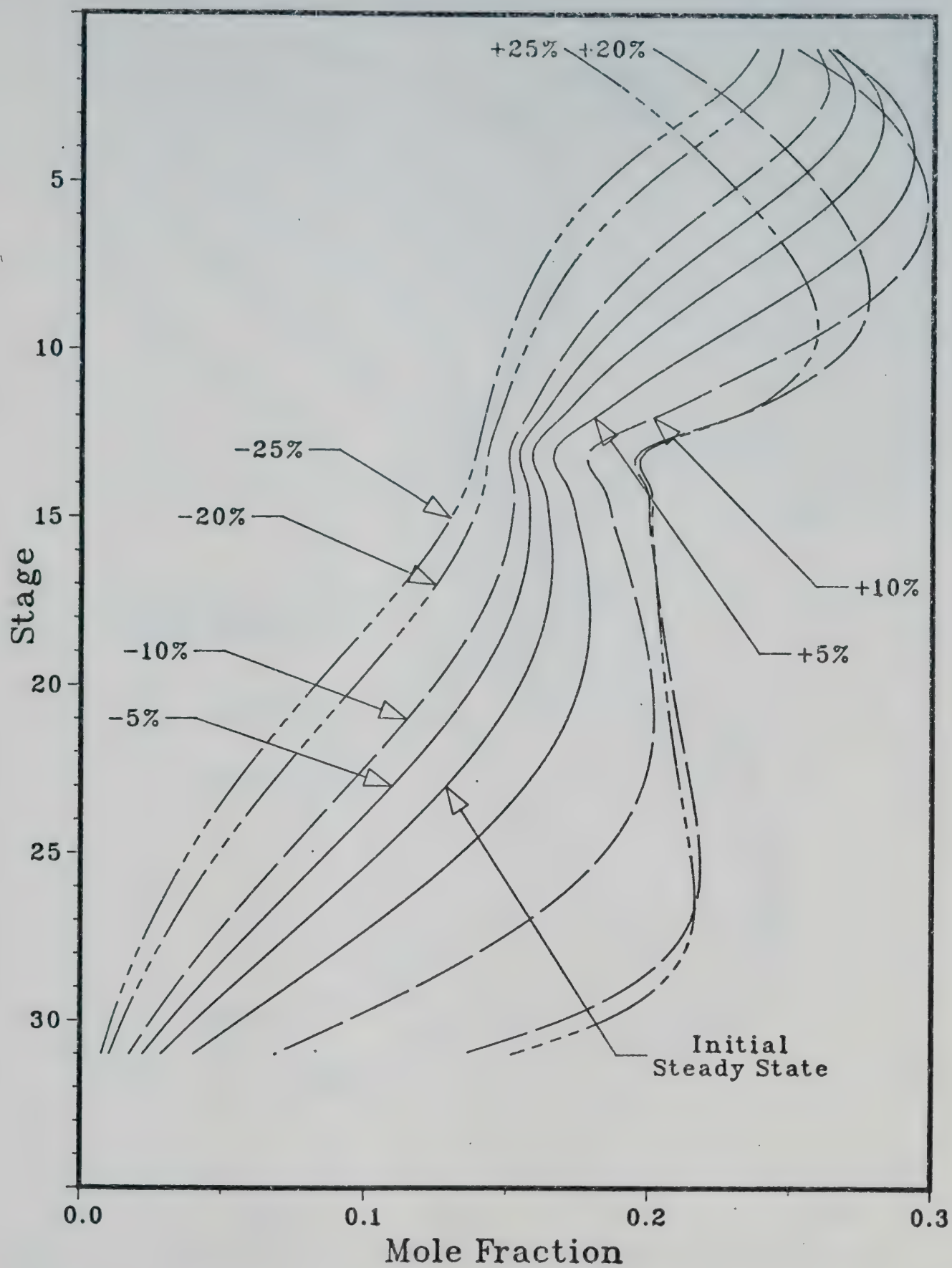


Fig. 4.12 Steady State Light Key Composition Profiles for Reflux Flow Rate Changes

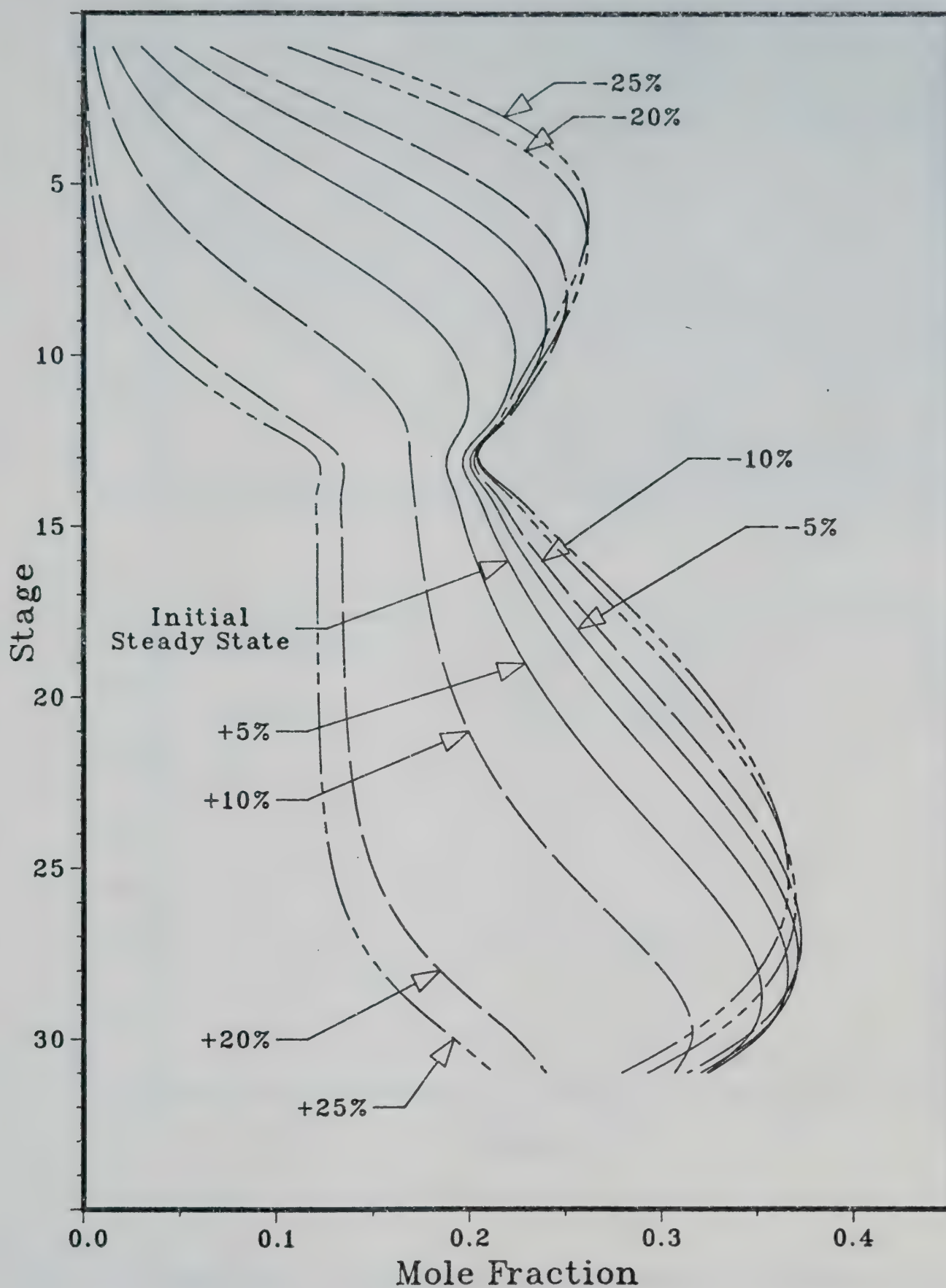


Fig. 4.13 Steady State Heavy Key Composition Profiles for Reflux Flow Rate Changes

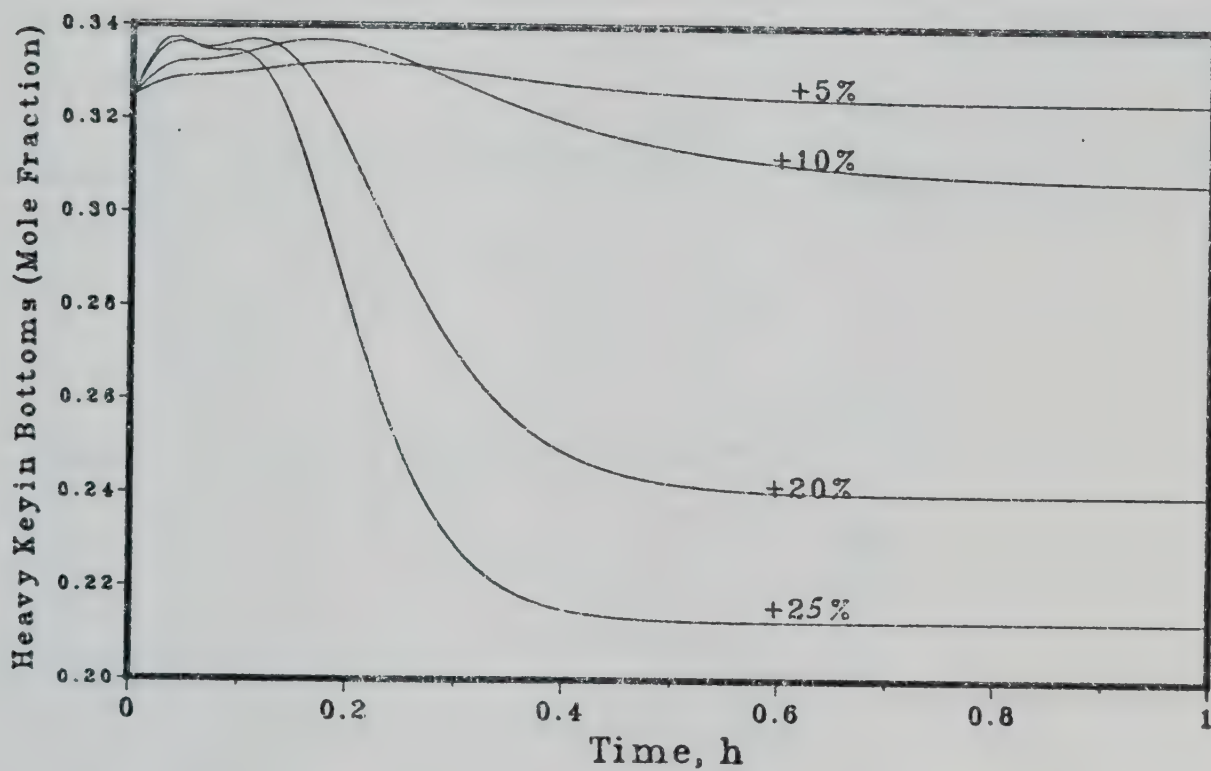
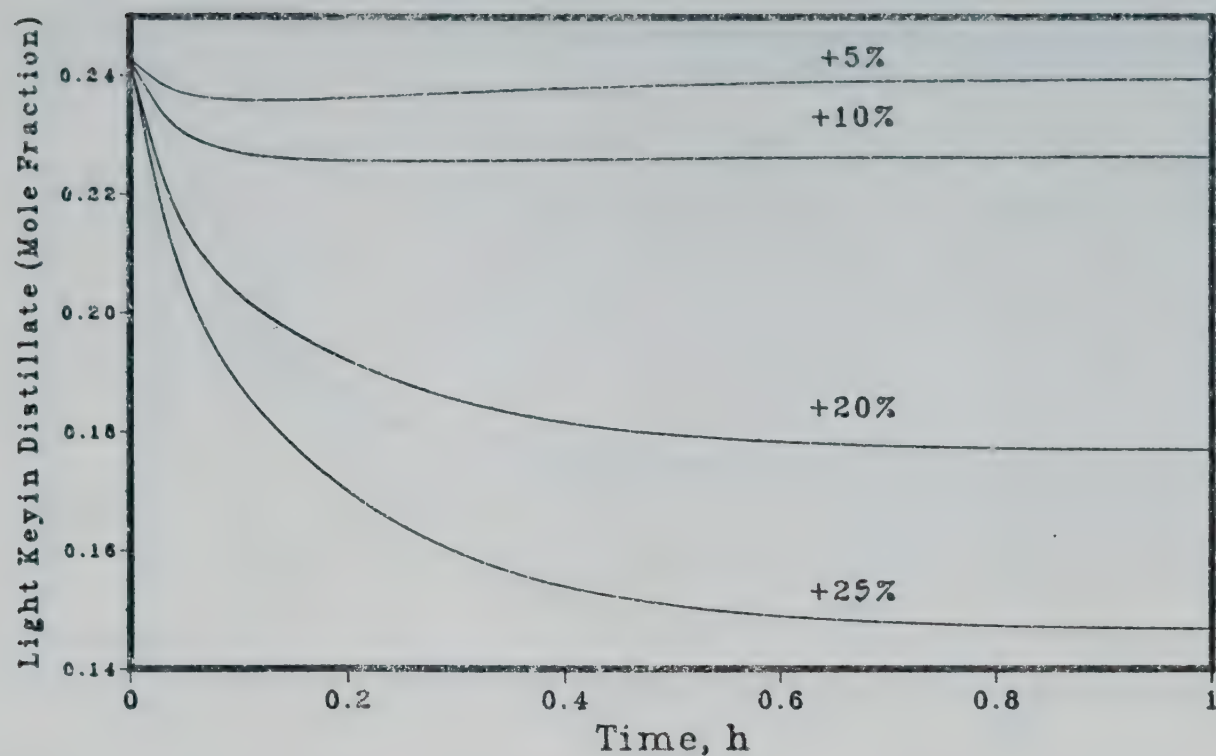


Fig. 4.14 Response of Product Compositions to Increases in Reflux Flow Rate

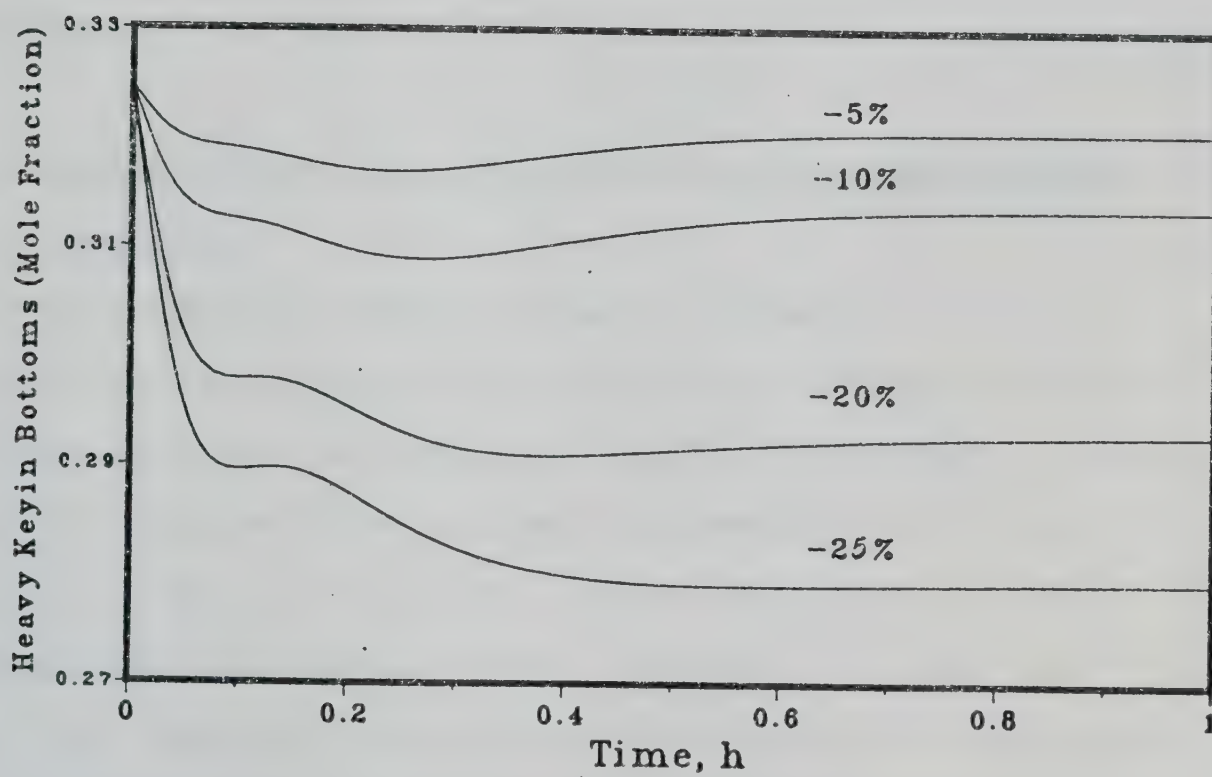
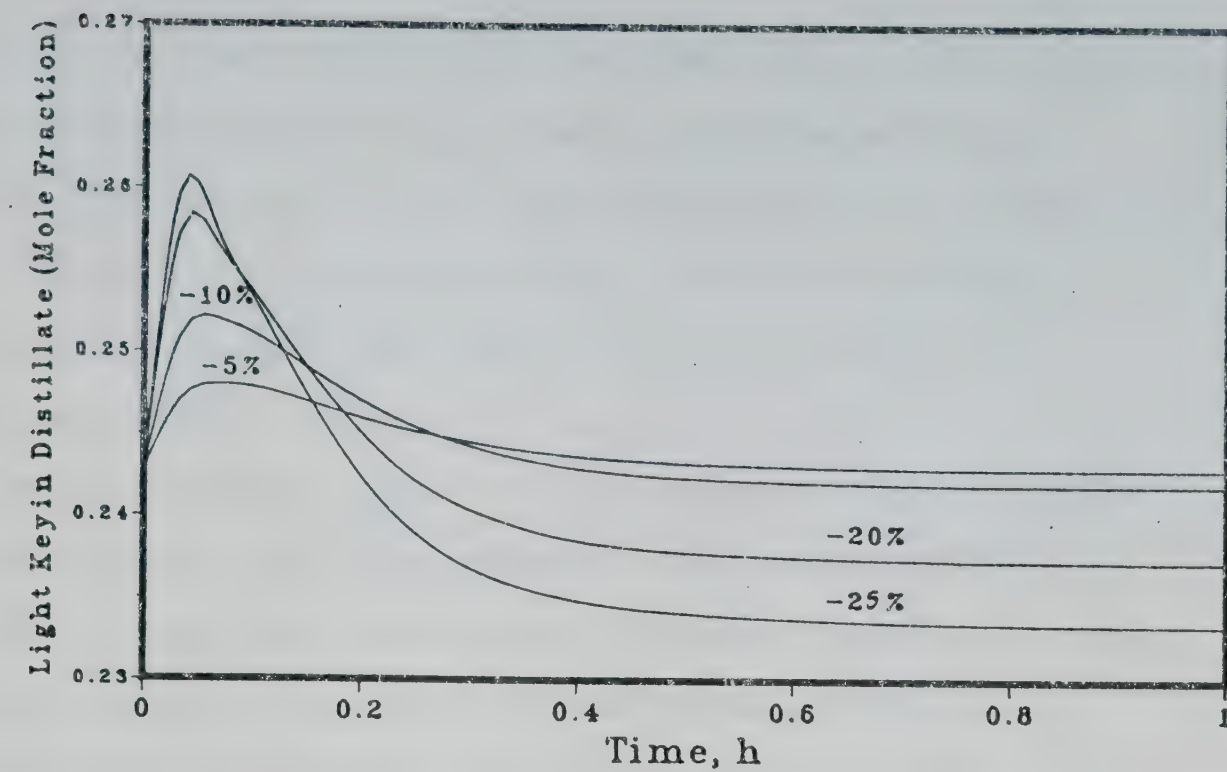


Fig. 4.15 Response of Product Compositions to Decreases in Reflux Flow Rate

For all the reflux flow rate tests none of the stage temperatures displayed any inverse response behavior. However the change in ethane composition in a few stages in the enriching section does exhibit inverse behavior, especially when the magnitude of the disturbance is relatively small.

The simulation results for the step changes in reflux flow rate agree with the behavior observed by Stathaki et al(26) in that the composition of the key component in the product streams can exhibit inverse response when the component is not present as impurity, as discussed in the beginning of this chapter.

4.1.4 Summary of the Dynamic Behavior of the Hydrocarbon Separator

The simulation results clearly indicate that the hydrocarbon separator can exhibit inverse response behavior in response to certain types of input disturbances. Inverse response is shown to be a common phenomenon in the key component compositions in the product streams when the component is not present in low concentration, eg. as impurity. However, for certain disturbances the composition of the impurities can exhibit inverse behavior as well. Furthermore inverse behavior can also be found in the liquid compositions on some of the intermediate trays.

These observations are consistent with the results reported by Stathaki et al(26). However in this work, the

temperature of some stages at and above the feed plate also exhibit inverse response to feed rate changes.

To illustrate the frequency of occurrence of inverse response in a concise manner, Tables 4.8 to 4.10 are the inverse response "maps" for each different type of disturbance investigated. These computer generated maps indicate the temperature or composition variables having inverse response on each stage. Inverse response is reported by the computer if the initial slope of a variable differs in sign from the final steady state gain of the variable.

Asymmetry in response time, on the other hand, is not as apparent in these simulation results as the results reported by Stathaki et al(26). In Table 4.11 the response time of some selected temperatures are listed with respect to the magnitude of the disturbances. The definition of response time, consistent with that used by Stathaki et al(26), is taken to be the time for a variable to be within 5% of the final steady state value and remain within this limit.

As can be seen from Table 4.11 the sign of the disturbance does not have a strong influence on the response time. Stathaki and co-workers(26) pointed out that the slow column dynamics seemed to be related to large shifts in the steady state temperature profile and the steady state distribution of the key components. However, the results in this work show that although the shift in steady profiles is

Table 4.8

Inverse Response Map for Feed Flow Rate Changes

+5% Change

-5% Change

STAGE	TEMP	COMPONENT				
		1	2	3	4	5
1	T	*	*	*	.	.
2	.	*	*	*	.	.
3	.	.	*	.	.	.
4	.	.	*	.	.	.
5	.	.	*	.	.	.
6	.	.	*	.	.	.
7	.	.	*	.	*	.
8	T	.	*	.	*	.
9	T	.	*	.	*	.
10	T	.	*	.	.	.
11	T	.	*	.	.	.
12	T	.	*	.	.	.
13	T	.	*	.	.	*
14	.	.	.	.	.	*
15	.	.	.	*	.	*
16	.	.	.	*	.	*
17	.	.	.	*	.	.
18	.	.	.	.	.	.
19	.	.	.	.	.	.
20	.	.	.	.	.	.
21	.	.	.	.	.	.
22	.	.	.	.	.	.
23	.	.	.	.	.	.
24	.	.	.	.	.	.
25	.	.	.	.	.	.
26	.	.	.	.	.	.
27	.	.	.	.	.	.
28	.	.	.	.	.	.
29	.	.	.	.	*	.
30	.	.	.	.	*	.
31	.	.	.	.	*	.

STAGE	TEMP	COMPONENT				
		1	2	3	4	5
1	T	*	*	*	.	.
2	T	*	*	*	.	.
3	T	.	*	.	.	.
4	T	.	*	.	*	.
5	T	.	*	.	*	.
6	T	.	*	.	*	.
7	T	.	*	.	*	.
8	T	.	*	.	*	.
9	T	.	*	.	*	.
10	T	.	*	.	.	.
11	T	.	*	.	.	*
12	T	.	*	*	.	*
13	T	.	*	*	.	*
14	.	.	.	*	.	*
15	.	.	.	*	.	*
16	.	.	.	*	.	*
17	.	.	.	*	.	.
18	.	.	.	.	.	.
19	.	.	.	.	.	.
20	.	.	.	.	.	.
21	.	.	.	.	.	.
22	.	.	.	.	.	.
23	.	.	.	.	.	.
24	.	.	.	.	.	.
25	.	.	.	.	.	.
26	.	.	.	.	.	.
27	.	.	.	.	.	.
28	.	.	.	.	.	.
29	.	.	.	.	*	.
30	.	.	.	.	*	.
31	.	.	.	.	*	.

* - COMPOSITION INVERSE RESPONSE
T - TEMPERATURE INVERSE RESPONSE
. - NORMAL RESPONSE

Table 4.9

Inverse Response Map for Heat Input Changes

+5% Change

-5% Change

STAGE	TEMP	COMPONENT					STAGE	TEMP	COMPONENT				
		1	2	3	4	5			1	2	3	4	5
1	.	.	.	*	.	.	1	.	.	.	.	.	.
2	.	.	.	*	.	.	2	.	.	.	.	.	.
3	.	.	.	.	.	.	3	.	.	.	*	.	.
4	.	.	.	.	.	.	4	.	.	.	.	.	.
5	.	.	.	.	.	.	5	.	.	.	.	.	.
6	.	.	.	.	.	.	6	.	.	.	.	.	.
7	.	.	.	.	.	.	7	.	.	.	.	.	.
8	.	.	.	.	.	.	8	.	.	.	.	.	.
9	.	.	.	.	.	.	9	.	.	.	.	.	.
10	.	.	.	.	.	.	10	.	.	.	.	.	.
11	.	.	.	.	.	.	11	.	.	.	.	.	.
12	.	.	.	.	.	.	12	.	.	.	.	.	.
13	.	.	.	.	.	.	13	.	.	.	.	.	.
14	.	.	.	.	.	.	14	.	.	.	.	.	.
15	.	.	.	.	.	.	15	.	.	.	.	.	.
16	.	.	.	.	.	.	16	.	.	.	.	.	.
17	.	.	.	.	.	.	17	.	.	.	.	.	.
18	.	.	.	.	.	.	18	.	.	.	.	.	.
19	.	.	.	.	.	.	19	.	.	.	.	.	.
20	.	.	.	.	.	.	20	.	.	.	.	.	.
21	.	.	.	.	.	.	21	.	.	.	.	.	.
22	.	.	.	.	.	.	22	.	.	.	.	.	.
23	.	.	.	.	.	.	23	.	.	.	.	.	.
24	.	.	.	.	.	.	24	.	.	.	.	.	.
25	.	.	.	.	.	.	25	.	.	.	.	.	.
26	.	.	.	.	.	.	26	.	.	.	.	.	.
27	.	.	.	.	.	.	27	.	.	.	.	.	.
28	.	.	.	.	.	.	28	.	.	.	.	.	.
29	.	.	.	.	*	.	29	.	.	.	.	.	.
30	.	.	.	.	*	.	30	.	.	.	.	*	.
31	.	.	.	.	.	.	31	.	.	.	.	*	.

* - COMPOSITION INVERSE RESPONSE
 T - TEMPERATURE INVERSE RESPONSE
 . - NORMAL RESPONSE

Table 4.10

Inverse Response Map for Reflux Flow Rate Changes

+5% Change

-5% Change

STAGE	TEMP	COMPONENT				
		1	2	3	4	5
1	.	.	.	.	.	.
2	.	.	.	*	.	.
3	.	.	.	*	.	.
4	.	.	.	.	.	.
5	.	*	.	.	.	.
6	.	*	.	.	.	.
7	.	*	.	.	.	.
8	.	*	.	.	.	.
9	.	*	.	.	.	.
10	.	*	.	.	.	.
11	.	*	.	.	.	.
12	.	.	.	.	*	.
13	.	*	.	.	*	.
14	.	.	.	.	.	.
15	.	.	.	.	.	.
16	.	.	.	.	.	.
17	.	.	.	.	.	.
18	.	.	.	.	.	.
19	.	.	.	.	.	.
20	.	.	.	.	.	.
21	.	.	.	.	.	.
22	.	.	.	.	.	.
23	.	.	.	.	.	.
24	.	.	.	.	.	.
25	.	.	.	.	.	.
26	.	.	.	.	.	.
27	.	.	.	.	.	.
28	.	.	.	.	.	.
29	.	.	.	.	.	.
30	.	.	.	.	*	.
31	.	.	.	.	*	.

STAGE	TEMP	COMPONENT				
		1	2	3	4	5
1	.	.	.	*	.	.
2	.	.	.	*	.	.
3	.	.	.	.	.	.
4	.	.	.	.	.	.
5	.	*	.	.	.	.
6	.	*	.	.	.	.
7	.	*	.	.	.	.
8	.	*	.	.	.	.
9	.	*	.	.	.	.
10	.	*	.	.	.	.
11	.	.	.	.	*	.
12	.	*	.	.	*	.
13	.	.	.	.	*	.
14	.	.	.	.	.	.
15	.	.	.	.	.	.
16	.	.	.	.	.	.
17	.	.	.	.	.	.
18	.	.	.	.	.	.
19	.	*	.	.	.	.
20	.	*	.	.	.	.
21	.	.	.	.	.	.
22	.	.	.	.	.	.
23	.	.	.	.	.	.
24	.	.	.	.	.	.
25	.	.	.	.	.	.
26	.	.	.	.	.	.
27	.	.	.	.	.	.
28	.	.	.	.	.	.
29	.	.	.	.	*	.
30	.	.	.	.	.	.
31	.	.	.	.	.	.

* - COMPOSITION INVERSE RESPONSE
 T - TEMPERATURE INVERSE RESPONSE
 . - NORMAL RESPONSE

Table 4.11

Response Time of Selected Stage Temperatures, T_j

Feed Disturbance Response Time, h

T_j	Disturbance Magnitude							
	-30%	-20%	-10%	- 5%	+ 5%	+10%	+20%	+30%
T_1	.750	.850	.900	.517	.750	.700	.800	.417
T_{10}	.617	.667	.500	.567	.683	.733	.733	.367
T_{20}	.483	.350	.450	.517	.567	.550	.433	.350
T_{31}	.733	.667	.317	.417	.550	.567	.500	.417

Heat Input Disturbance Response Time, h

T_j	Disturbance Magnitude							
	-20%	-15%	-10%	- 5%	+ 5%	+10%	+15%	+20%
T_1	.100	.100	.133	.200	.200	.167	.167	.300
T_{10}	.267	.300	.367	.333	.167	.367	.367	.333
T_{20}	.267	.333	.400	.467	.133	.200	.167	.133
T_{31}	.367	.433	.500	.433	.433	.467	.467	.467

Reflux Rate Disturbance Response Time, h

T_j	Disturbance Magnitude							
	-25%	-20%	-10%	- 5%	+ 5%	+10%	+20%	+25%
T_1	.167	.133	.133	.133	.133	.100	.067	.100
T_{10}	.100	.233	.367	.367	.233	.400	.233	.167
T_{20}	.133	.133	.400	.433	.267	.500	.300	.233
T_{31}	.267	.200	.467	.500	.433	.633	.433	.333

often very nonlinear with respect to the magnitude of the input change, the response times remain comparable in magnitude for the same type of disturbance.

5. Simulation of a Pilot Scale Water-Methanol Binary Distillation Column

The distillation column considered in this chapter is a pilot scale column located in the Department of Chemical Engineering at the University of Alberta. The column has eight trays with a total condenser and a partial reboiler. Operating pressures for the column is about 1 atmosphere. Detailed design specifications of this column are given by Svrcek(31), but the specifications, pertinent to the simulation study, are listed in Table 5.1.

Although the column is only of pilot scale, an extensive amount of experimental data have been accumulated over the years of control system and dynamics studies, so is an excellent choice for comparison of simulation model predictions versus experimental data.

From an analysis of preliminary simulation results it was found that the basic model presented in Chapter 2 can only provide an approximation to the steady state and dynamic characteristics of this column. As a result the model discussed in chapter 2 is refined to provide a better representation of the actual process. The refinements made to the basic model are concerned with

- i. external heat loss
- ii. heat transfer inside the reboiler
- iii. tray efficiencies.

In this chapter, the discussion is devoted mainly to the refinements incorporated into the model and the

Table 5.1
Partial Specification of the Binary Column

Components: $\text{H}_2\text{O}(1) - \text{CH}_3\text{OH}(2)$
Column Pressure: 1 atm.
Feed tray: 5th from top tray (stage 6)
Feed composition (mole %): $x_1 = 63.6$, $x_2 = 36.4$
Feed temperature: 334 K
Condenser coolant: Water at 284 K
Reboiler heating medium: saturated steam at 392 K
Tray area: 413 cm^2
Equivalent weir width: 7.5 cm
Weir height: 5.0 cm

simulation results obtained from using the modified model.

5.1 Refinement of the Basic Model

5.1.1 External Heat Loss

Because of exposure to the environment and the lack of insulation, the column is subject to heat loss. As a first approximation, the heat loss from each tray can be assumed to be constant despite disturbances to the column. However, it is more appropriate to incorporate a variable heat loss representation into the model to allow the heat loss to change during the transient. The heat loss model used in

this simulation, based on an overall heat transfer coefficient between the tray liquid on stage j and the environment, was

$$Q_j = UA_j (T - T_j) \quad (5.1)$$

where T_j is the tray temperature and T is the ambient temperature, assumed constant. The product of the overall heat transfer coefficient and the heat transfer area for each tray and for the reboiler and the condenser, UA_j , is allowed to vary from stage to stage but is constant with respect to time. The experimental data show that more than 10% of the heat input is lost to the ambient.

5.1.2 Reboiler Heat Load

The reboiler heat load of the column can vary to a certain degree because the effectiveness of the heat exchanger is dependent on the temperature gradient between the reboiler liquid and the input steam. It is therefore natural to model the heat input using a heat transfer approach analogous to equation 5.1, that is

$$Q_r = UA_r (T_{s,t} - T_n) \quad (5.2)$$

The equilibrium temperature of the reboiler liquid, T_n , will vary in the transient phase, furthermore the steam temperature, although assumed constant in the simulation,

can be variable if the dynamic behavior of the steam chest is considered. The heat transfer expression, equation 5.2, however, was found to be inadequate to describe the heat exchange process inside the reboiler after performing some trial simulations of the column. The failure of equation 5.2 to accurately describe the behavior was due to the assumption that UAr was constant. However, UAr varied possibly because

- i. as the equilibrium temperature in the reboiler decreased as the liquid contained more of the volatile component, the effective heat transfer area was reduced by the bubbles formed on the heat transfer surface;
- ii. as the equilibrium temperature in the reboiler decreased and the condensed water film on the steam side grew in thickness, the effective heat exchange was also reduced.

The simulation results seem to support consistently the above reasons. For example, as the temperature of the reboiler liquid decreases, the temperature difference between the liquid and the steam is increased so if UAr were constant, as is in equation 5.2, the computed Q_r would be considerably more than that was actually delivered by the amount of steam consumed.

In order to model the heat input rate so that its value is closer to the value measured from the experiment, UAr is allowed to vary in the following manner

$$UAr = UAr(initial) + Cr[T_n(t) - T_n(initial)] \quad (5.3)$$

where the subscript i denotes a value from the initial steady state. Equation 5.3 represents the variation of UAr as a perturbation from the initial steady state value. The sensitivity of UAr to temperature change is governed by the empirical coefficient Cr.

5.1.3 Tray Efficiency

The results of some simulation trial tests strongly indicate that the tray efficiencies have a significant influence on the steady state solution and the transient behavior of the simulation. In order to obtain satisfactory agreement between the computed response and the measured response, it is necessary to vary the overall tray efficiency with some empirical relationship.

A rather simple form of correlation, used by Simonsmeier(29) in the simulation of the same column, is the following

$$\zeta = \frac{E_m(\text{final}) - E_m(\text{initial})}{x(\text{final}) - x(\text{initial})} \quad (5.4)$$

where x denotes the composition of a selected component at a selected stage, with the overall tray efficiency expressed as follows

$$E_m = \zeta[x(t) - x(\text{initial})] + E_m(\text{initial}) \quad (5.5)$$

Equations 5.3 and 5.5, although written in different forms, employ the same basic concept, in which the variation during transient operation is approximated as a linearized perturbation around the initial steady state.

The empirical correlations in equations 5.3 and 5.5 are very simple and easy to incorporate into the dynamic simulator. However it suffers from the fact that tray efficiencies are generally not strong functions of compositions, so tray composition is really not a desirable variable for use in such a correlation. In simulation tests using this correlation, it was found that although the computed values of the different variables can be matched with the measured values at steady state, the transient response values do not agree satisfactorily with the experimental results.

On the basis of mass transfer considerations, it is more reasonable to correlate the overall tray efficiency with the liquid and vapor flow rates, since these are the determining variables for contact time of the two phases. For the average flow rates defined as

$$\bar{V} = \frac{\sum_j V_j}{(n-1)} \quad j = 2, 3, \dots, n \quad (5.6)$$

$$\bar{L} = \frac{\sum_j L_j}{(n-1)} \quad j = 2, 3, \dots, n \quad (5.7)$$

a weighted average rate can be computed as

$$\theta = \eta \bar{L} + (1-\eta) \bar{V} \quad 0 \leq \eta \leq 1 \quad (5.8)$$

Then using a linear approach, as in equation 5.5, the efficiency correlation may be written as

$$\xi = \frac{E_m(\text{final}) - E_m(\text{initial})}{\theta(\text{final}) - \theta(\text{initial})} \quad (5.9)$$

$$E_m = \xi[\theta(t) - \theta(\text{initial})] + E_m(\text{initial}) \quad (5.10)$$

Use of this form of empirical correlation resulted in a much improved agreement between the computed results and the experimental results, as will be shown in the later sections.

5.2 Simulation of Steady States for Feed Rate Changes

Before simulating the transient response, the dynamic simulator was used to compute the initial steady state. Since all of the streams entering or leaving the column are closely monitored during experimentation, the accurate values are known and can be used as parameters in the simulation. The parameters that cannot be measured directly and yet play important roles in the computation of steady states are the external heat loss, the overall heat transfer coefficient for the inside of the reboiler and the tray efficiencies. However with the available experimental data it is possible to obtain estimates of these parameters so that the simulated steady state conditions agree with the

experimental data. The reboiler heat duty, although not directly measured, can be estimated from the enthalpy and the rate of condensation of the input steam. From this estimate, the overall heat transfer coefficient can be calculated. The tray heat loss may be estimated from an overall energy balance. This estimate can be used to calculate an approximate value of the external heat transfer coefficient. The tray efficiency has previously been estimated by Svrcek(31), but the values, which ranged from 40% to over 100%, were not considered reliable, therefore the tray efficiency is the parameter with the most uncertainty. By varying the parameters, the simulated steady state can be matched with the experimental results, but matching is an iterative process so can only be easily performed by computer.

5.2.1 Feed Rate Disturbances

The column experimental data used for model verification was that obtained by Vagi(27). The test data selected was that obtained from test number FEED10 for the change in feed flow rate, as shown in Figure 5.1, so that the operating regions above and below the steady state operation could be explored. The experiment thus involves four distinct transient phases with the feed rates as given in Table 5.2. A comparison of some of the computed and experimental steady state values of the variables are listed in Tables 5.3 to 5.6. Table 5.7 is a list of the parameters

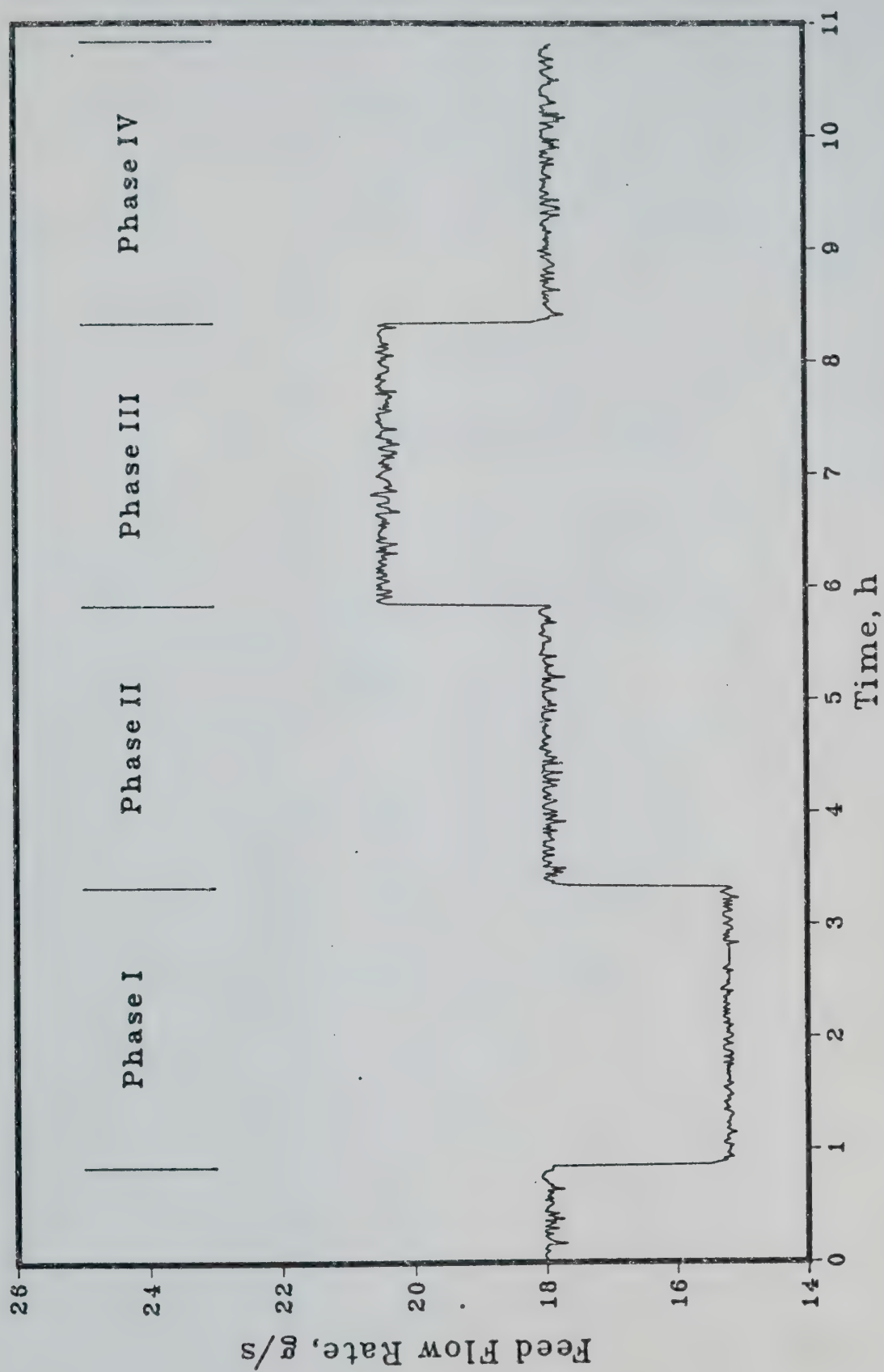


Fig. 5.1 Feed Flow Rate Disturbance to Water-Methanol Column.

Table 5.2
Average Feed rates

Phase	Feed (mol/s)
Steady State	0.777
I	0.658 (-15%)
II	0.777 (+18%)
III	0.883 (+14%)
IV	0.777 (-12%)

Table 5.3

Comparison of Predicted Steady State Data of Phase I for
 $Cr = 3.383 \text{ E-5 kW/K}^2$ with Experimental Data

	Initial		Final	
	Sim.	Exp.	Sim.	Exp.
<u>Top Product:</u>				
Mole % MeOH	91.92	91.92	91.16	91.16
Flow rate(mol/s)	.2873	.232	.2595	.215
Temp. (K)	338.9	336.1	339.0	336.5
<u>Bot. Product:</u>				
Mole % MeOH	3.74	3.74	0.57	0.57
Flow rate(mol/s)	.4896	.548	.3970	.452
Temp. (K)	368.4	364.0	372.3	368.9
Qr (kW)	22.60	19.5	21.73	19.2
UAr (kW/K)	.9175	—	1.052	—
Qc (kW)	-18.68	-16.1	-17.78	-15.7
Total Heat loss(kW)	-2.71	-2.1	-2.89	-2.4
E _m	0.766	—	0.869	—

Table 5.4

Comparison of Predicted Steady State Data of Phase II for
 $Cr = 3.437 \text{ E-5 kW/K}^2$ with Experimental Data

	Initial		Final	
	Sim.	Exp.	Sim.	Exp.
<u>Top Product:</u>				
Mole % MeOH	91.14	91.16	91.83	91.82
Flow rate(mol/s)	.2598	.215	.2872	.232
Temp. (K)	339.0	336.5	338.9	336.1
<u>Bot. Product:</u>				
Mole % MeOH	0.56	0.57	3.82	3.82
Flow rate(mol/s)	.3983	.452	.4897	.548
Temp. (K)	372.4	368.9	368.3	363.8
Qr (kW)	21.75	19.2	22.58	19.5
UAr (kW/K)	1.053	—	0.914	—
Qc (kW)	-17.80	-15.7	-18.68	-16.1
Total Heat loss(kW)	-2.89	-2.4	-2.71	-2.1
E _m	0.871	—	0.759	—

Table 5.5

Comparison of Predicted Steady State Data of Phase III for
 $Cr = 2.500 \text{ E-5 kW/K}^2$ with Experimental Data

	Initial		Final	
	Sim.	Exp.	Sim.	Exp.
<u>Top Product:</u>				
Mole % MeOH	91.83	91.82	91.61	91.61
Flow rate(mol/s)	.2875	.232	.3072	.237
Temp. (K)	338.9	336.1	339.0	336.1
<u>Bot. Product:</u>				
Mole % MeOH	3.79	3.82	6.90	6.90
Flow rate(mol/s)	.4895	.548	.5762	.649
Temp. (K)	368.3	363.8	365.2	360.2
Qr (kW)	22.62	19.5	23.30	19.8
UAr (kW/K)	1.053	—	.913	—
Qc (kW)	-18.68	-16.1	-19.35	-16.5
Total Heat loss(kW)	-2.89	-2.1	-2.71	-2.0
E _m	0.760	—	0.734	—

Table 5.6

Comparison of Predicted Steady State Data of Phase IV for
 $C_r = 2.492 \text{ E-5 kW/K}^2$ with Experimental Data

	Initial		Final	
	Sim.	Exp.	Sim.	Exp.
<u>Top Product:</u>				
Mole % MeOH	91.60	91.61	91.67	91.67
Flow rate(mol/s)	.3075	.237	.2878	.233
Temp. (K)	339.0	336.1	339.0	336.1
<u>Bot. Product:</u>				
Mole % MeOH	6.90	6.90	3.74	3.74
Flow rate(mol/s)	.5762	.649	.4880	.548
Temp. (K)	365.2	360.2	368.4	363.7
Qr (kW)	23.33	19.8	22.62	29.5
UAr (kW/K)	0.838	—	.918	—
Qc (kW)	-19.35	-16.5	-18.70	-16.1
Total Heat loss(kW)	-2.65	-2.0	-2.72	-2.1
E _m	0.734	—	0.753	—

Table 5.7

Summary of Constant parameters in the simulationsColumn:

No. of stages = 10

Feed stage = 6

Column pressure = 101.3 kPa

Tray area(†) = 413 cm²

Equivalent weir width(†) = 7.5 cm

Weir height(†) = 5.0 cm

Reflux:

Reflux rate = 0.277 mol/s.

Feed stream:

Methanol mole fraction = 0.364

Feed temperature = 334. K

Feed pressure = 101.3 kPa

Heat loss:

Ambient temperature = 292 K

$UA_1 = 4.83 \text{ W/K}$

$UA_j = 3.83 \text{ W/K} \quad j = 2, 3, \dots, 9$

$UA_{10} = 9.67 \text{ W/K}$

Holdup(‡):

Condenser holdup = 23.4 mol

Reboiler holdup = 400 mol

(†) - Simonsmeier(29)

(‡) - Bilec(4)

held constant for all four transient phases of the simulation.

5.3 Simulation of the Transient Phases

The simulation results for each of the step changes were obtained using different overall tray efficiency correlations. Figure 5.2 is a plot of the response of the concentration of methanol in the top product during phase I of the transient response. The responses were obtained using an overall tray efficiency correlated with the composition of methanol on different stages. The test code numbers in the figure have the following meaning

BI.FD.OL11 - E_m correlated with composition on stage 6

BI.FD.OL13 - E_m correlated with composition on stage 7

BI.FD.OL14 - E_m correlated with composition on stage 5

It can be seen that using the composition on stage 6 yields the best match of the predicted response with the experimental data. However, as can be seen in Figure 5.3, which is a similar plot for the second phase of the complete transient, where

BI.FD.OL21 - E_m correlated with composition on stage 6

BI.FD.OL23 - E_m correlated with composition on stage 4

correlating the efficiency with the composition on stage 6

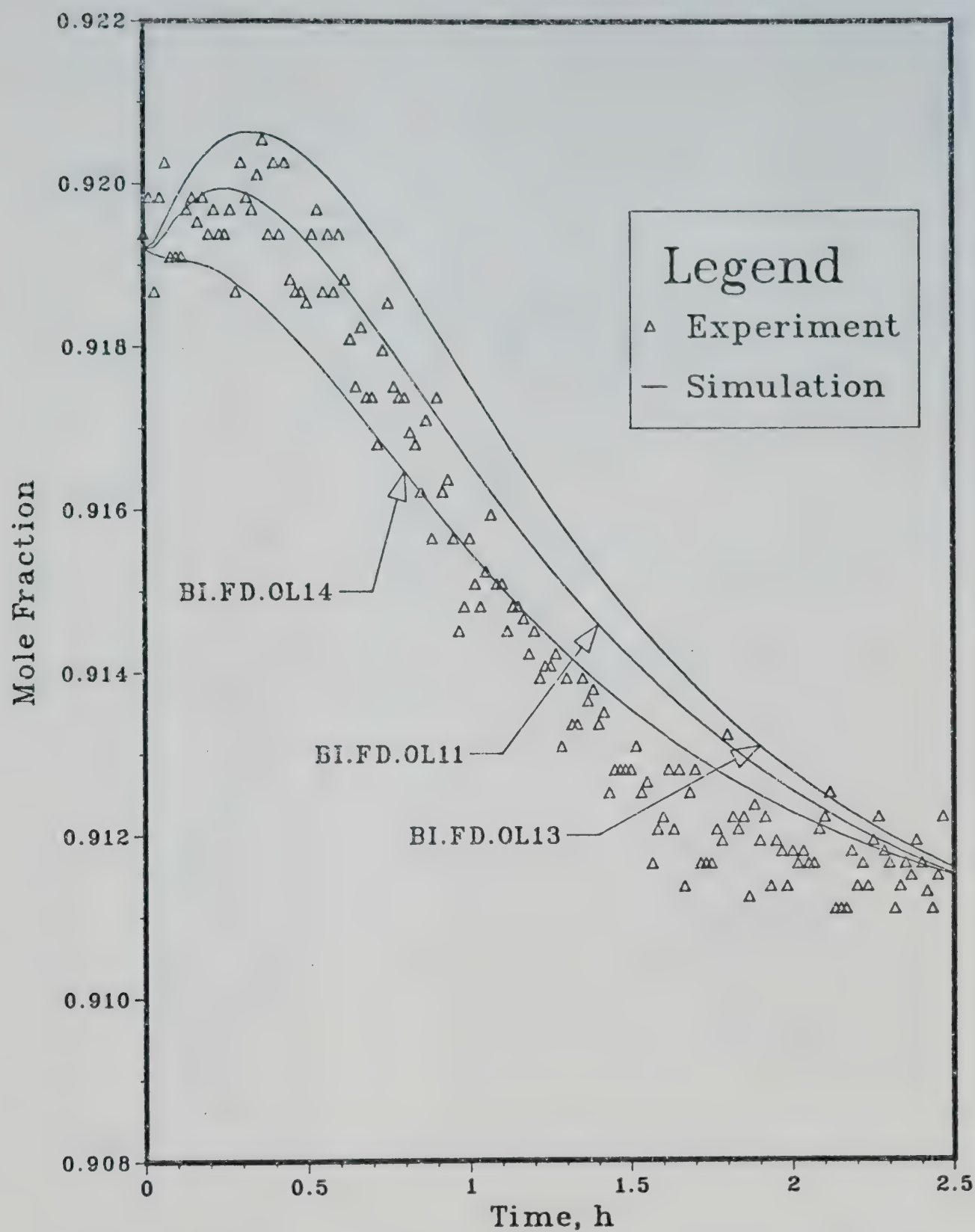


Fig. 5.2 Phase I Response of Methanol Composition in the Top Product Using E_m Correlated with Stage Composition.

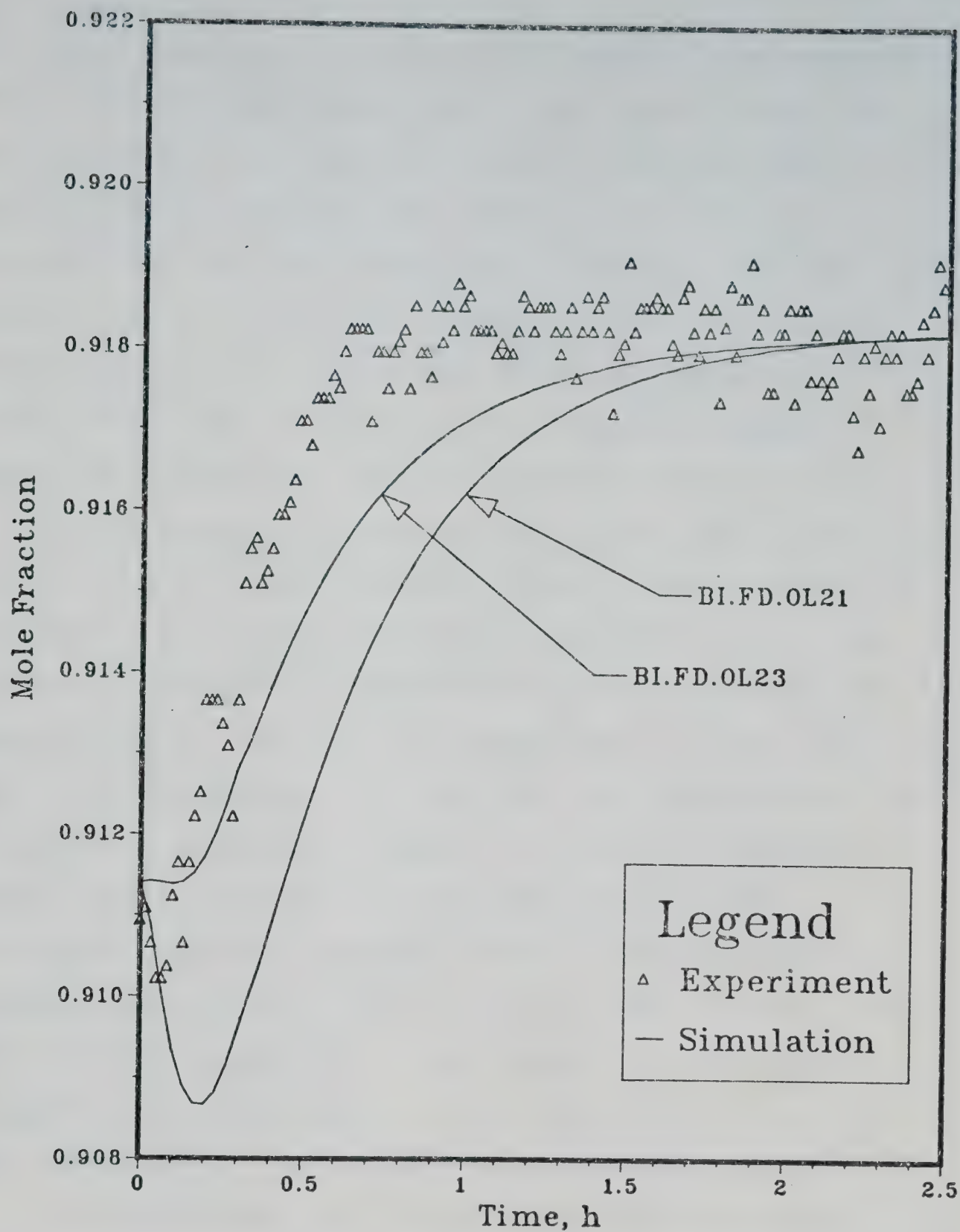


Fig. 5.3 Phase II Response of Methanol Composition in the Top Product Using E_m Correlated with Stage Composition.

no longer resulted in a satisfactory match of the predicted value with the experimental data. The results showed that the composition on stage 4 is a better choice as the correlating variable for this phase. It is therefore obvious that using the composition of any one stage for the correlation of the overall tray efficiency cannot always yield satisfactory results under different operating conditions. This is because the correlation is purely empirical and does not have any physical significance.

As an alternative approach the average vapor flow rate can be used as the correlating variable, that is, $\eta = 0$ in equation 5.8. The top composition response of phase I as plotted in Figure 5.4 matches well with the experimental data except for the inverse response behavior that occurs in the first few samples. On the other hand the predicted top composition response for phase II as shown in Figure 5.5 shows good to agreement with the experimental data throughout the whole transient phase. The bottom product composition response in both Figures 5.4 and 5.5 agree quite well with the experimental data, except that the computed response is slightly faster. This is probably because of the inaccuracy in the estimate of the reboiler holdup.

If the average liquid flow rate is used instead to correlate the overall tray efficiency, that is, $\eta = 1$, the predicted response would be quite different. As can be seen in Figure 5.6, the top product composition initially exhibits excessive inverse response behavior which also

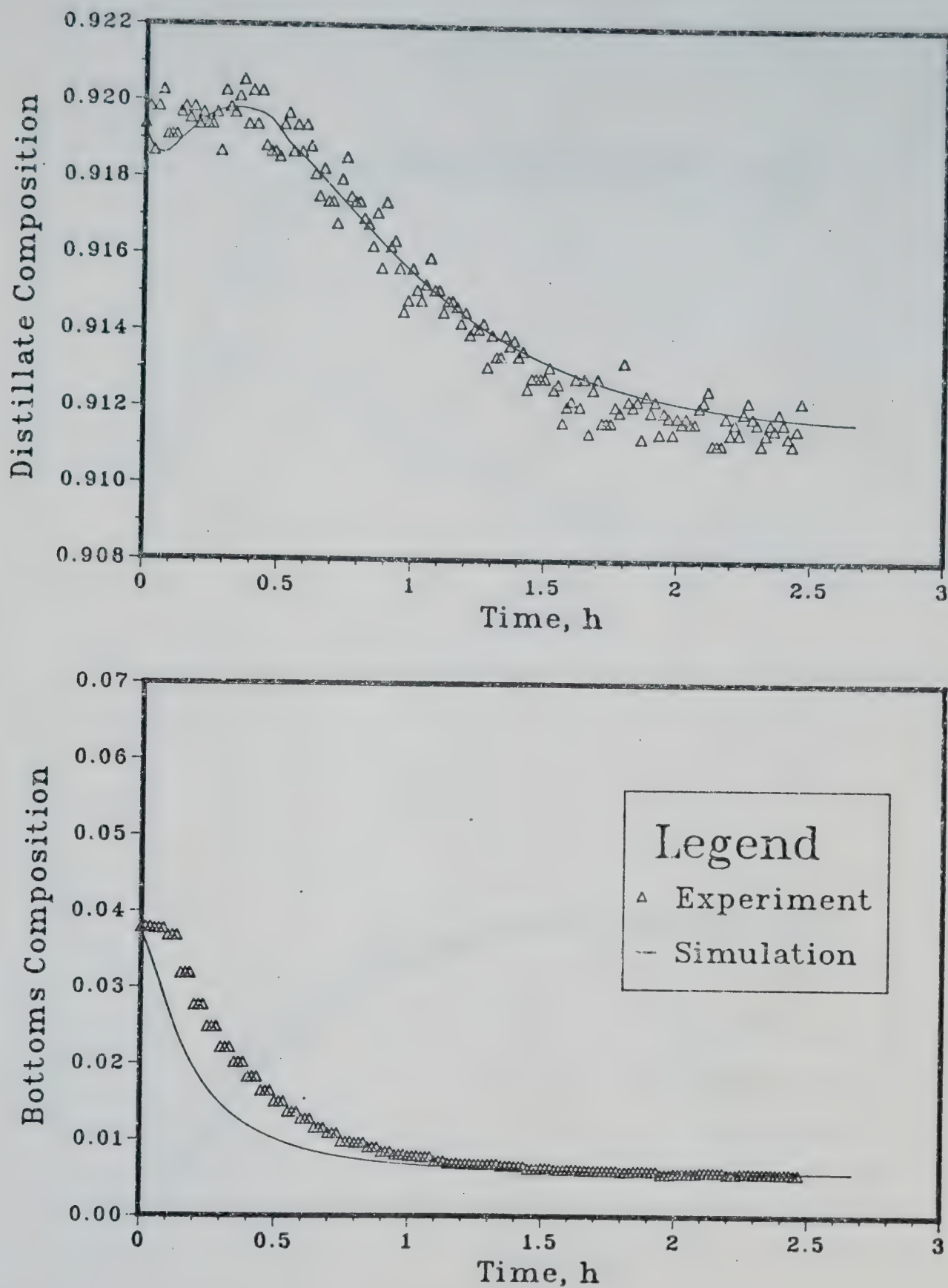


Fig. 5.4 Phase I Response of Methanol Composition in the Products Using E_m Correlated with Average Vapor Flow Rate.

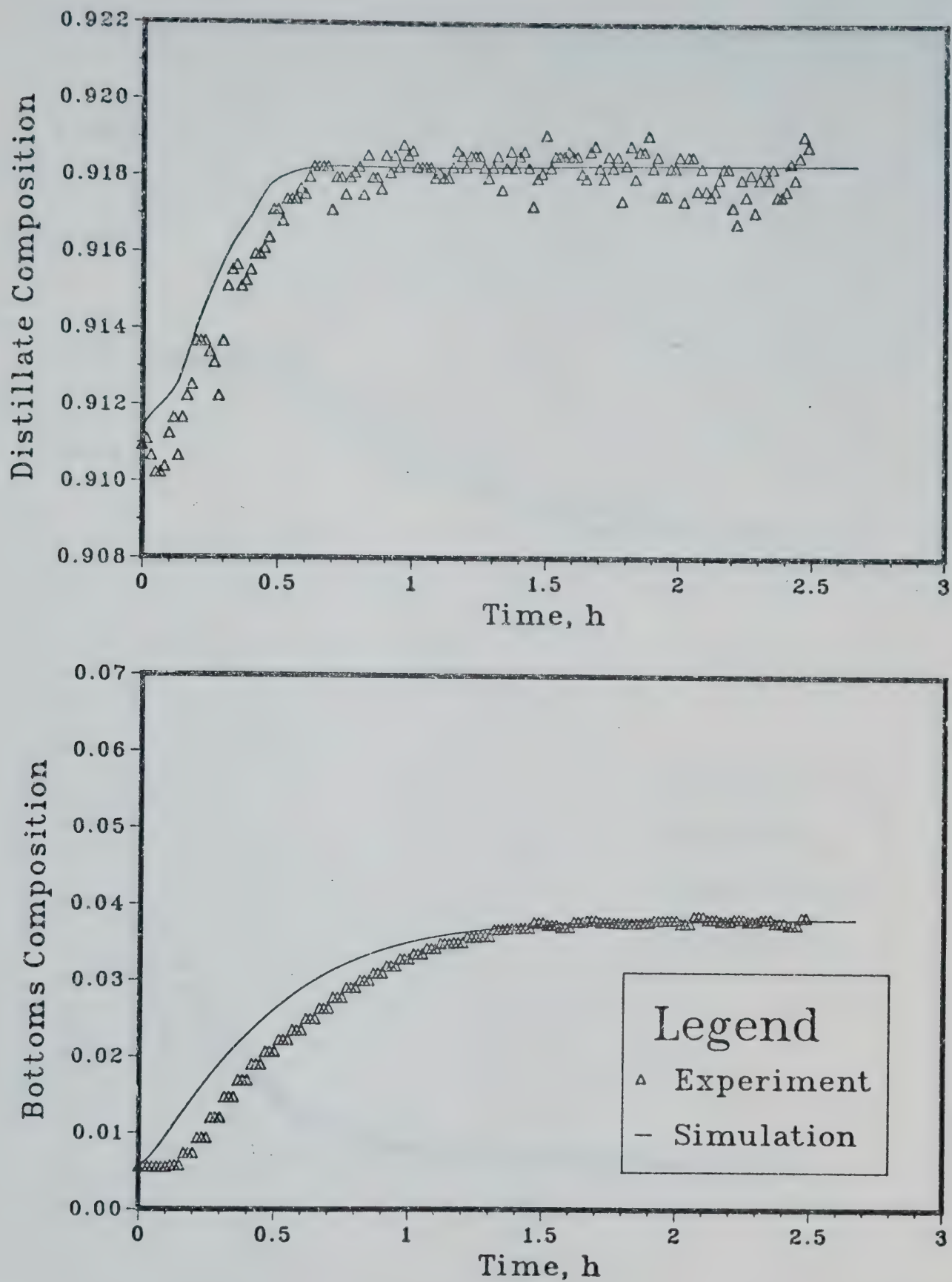


Fig. 5.5 Phase II Response of Methanol Composition in the Products Using E_m Correlated with Average Vapor Flow Rate.

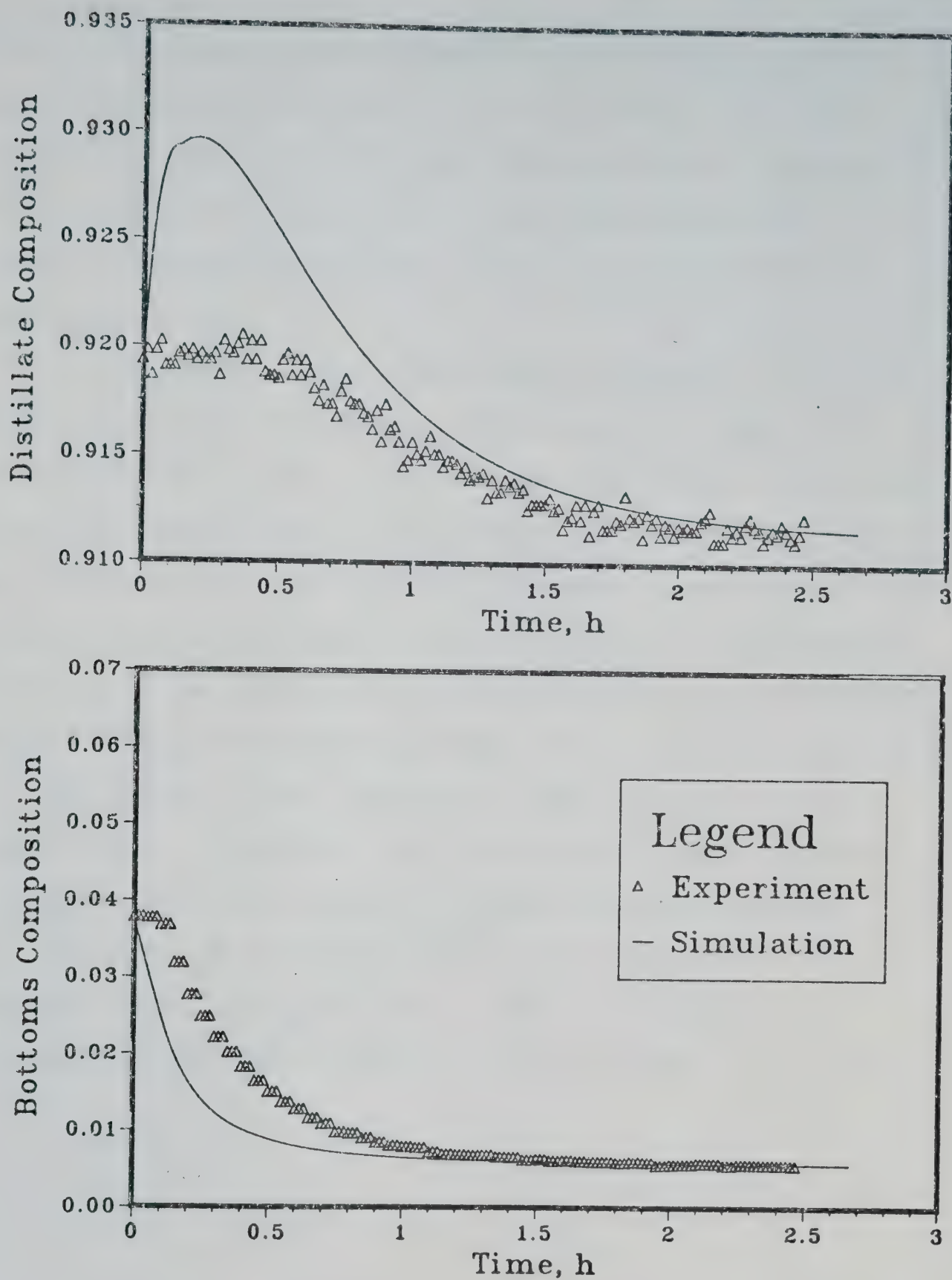


Fig. 5.6 Phase I Response of Methanol Composition in the Products Using E_m Correlated with Average Liquid Flow Rate.

affects the response trajectory for the remaining part of the transient period. Similar characteristics can be observed in Figure 5.7 in which the top product response is plotted for transient phase II. The simulation also predicts inverse response that cannot be found in the experimental data.

As the overall tray efficiency is actually a function of the flow rates of both the liquid and the vapor, it is more reasonable to set η between zero and unity. After some iterative computations, it was found that when η is around the value of 0.03 the simulated response becomes quite close to the experimental response for all phases of the complete transient. The predicted transient response of the methanol composition in the product streams for $\eta = 0.03$ are plotted for each phase of the transient in Figures 5.8 to 5.11 respectively. Therefore use of an overall tray efficiency correlated with equations 5.6 to 5.10 has the advantage that for the range of operating conditions η can be set to a constant value, and the need to select a stage or a composition for the correlation is eliminated.

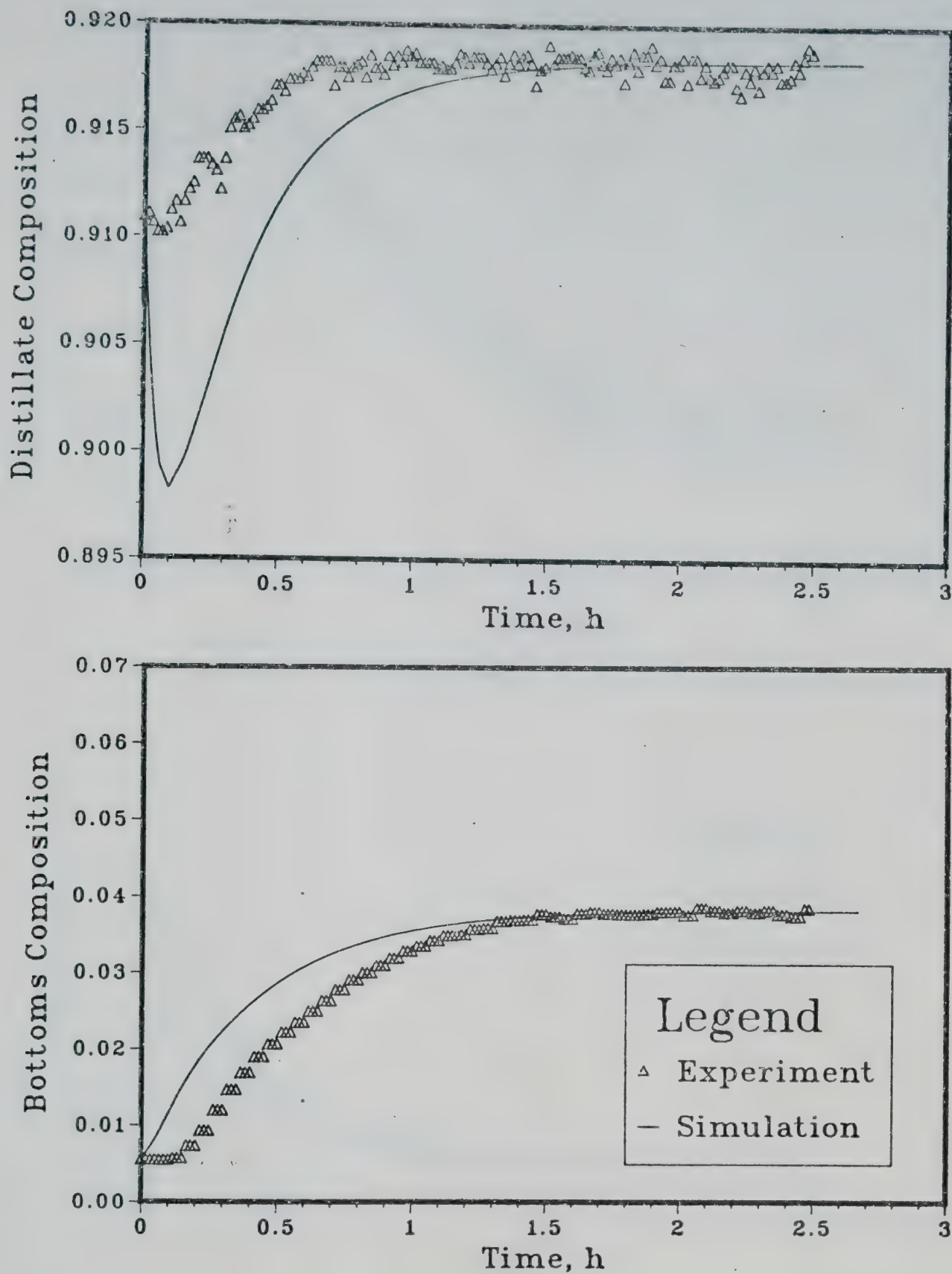


Fig. 5.7 Phase II Response of Methanol Composition in the Products Using E_m Correlated with Average Liquid Flow Rate.

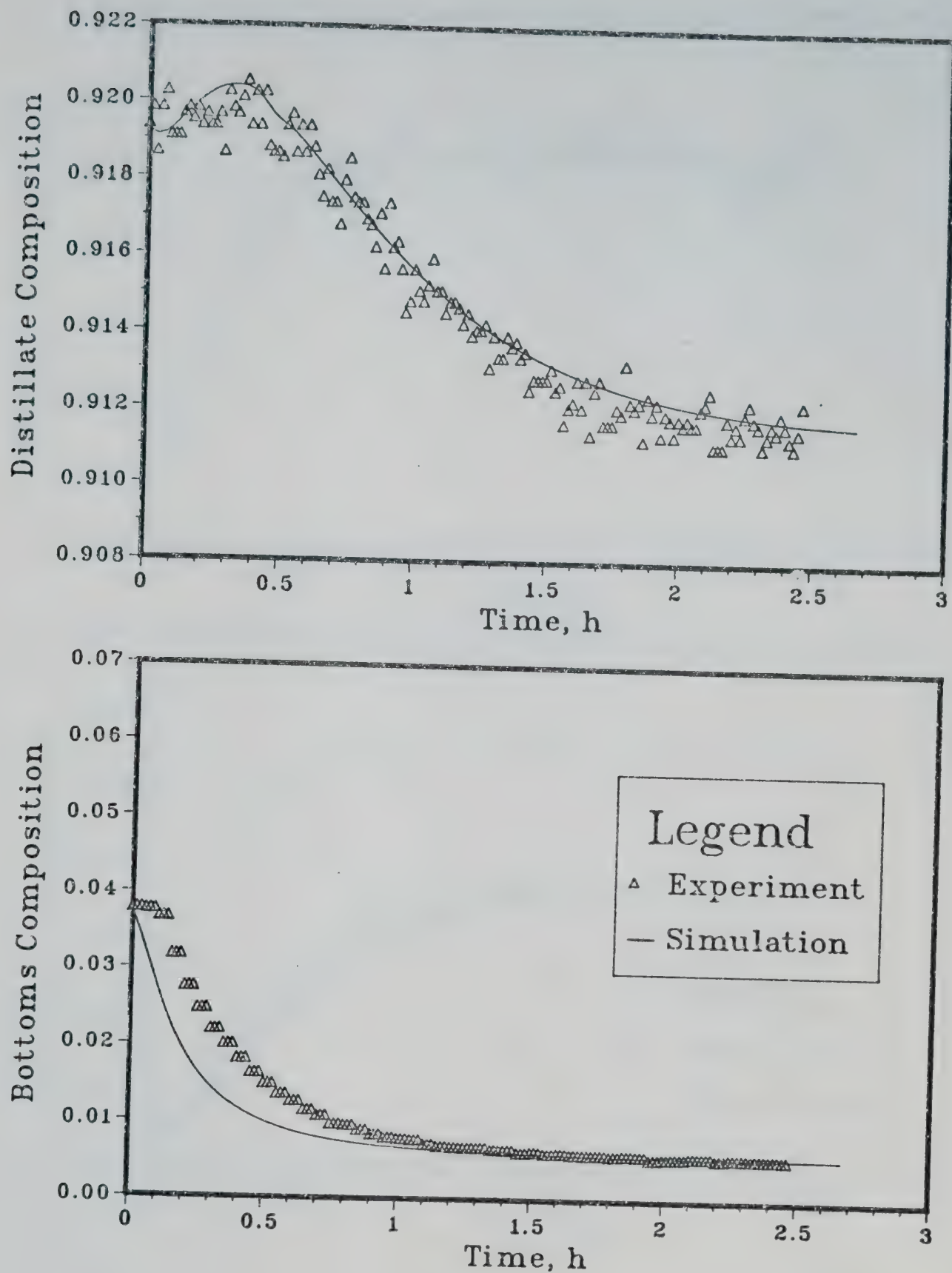


Fig. 5.8 Phase I Response of Methanol Composition in the Products Using E_m Correlated with $\eta = 0.03$.

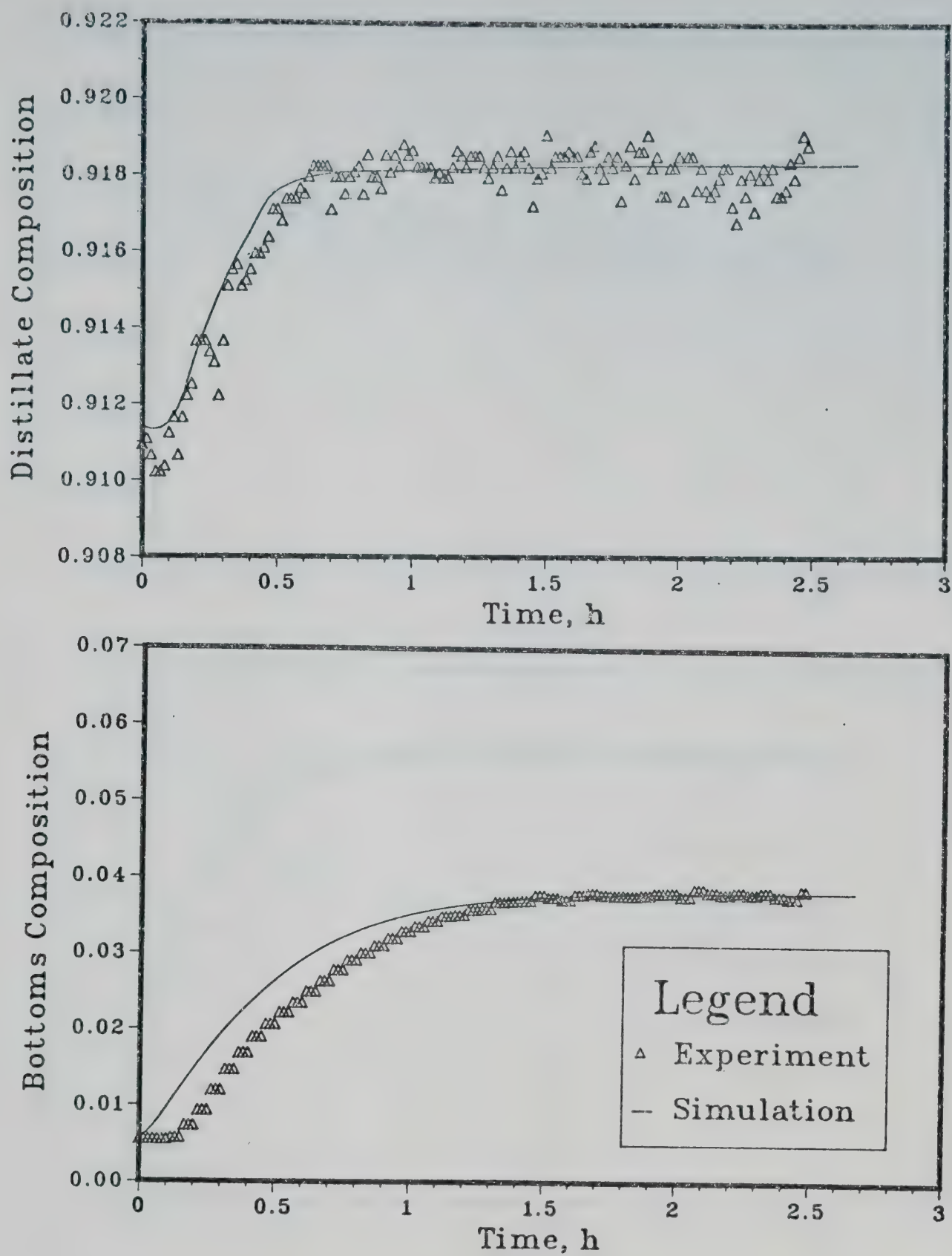


Fig. 5.9 Phase II Response of Methanol Composition in the Products Using E_m Correlated with $\eta = 0.03$.

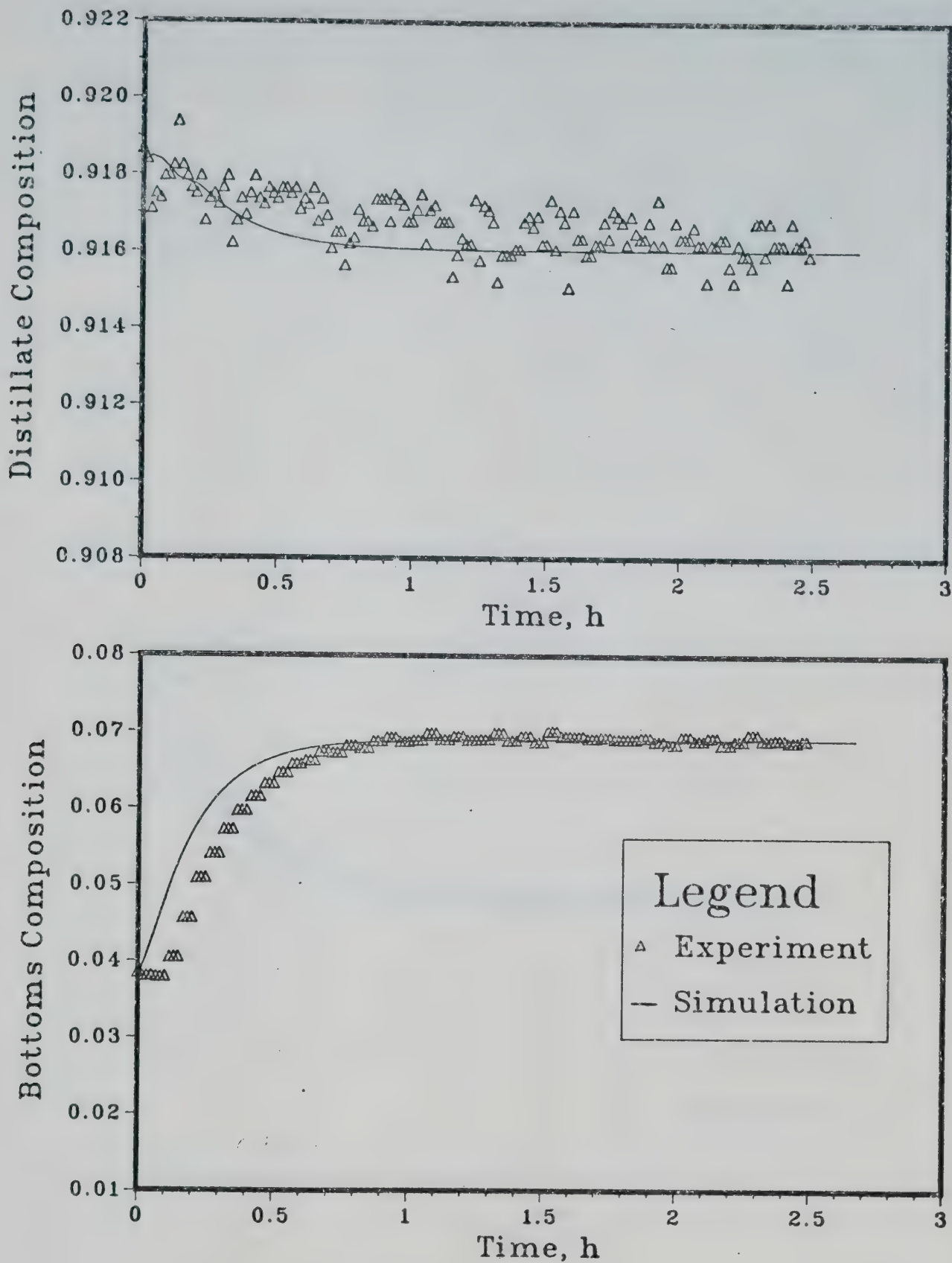


Fig. 5.10 Phase III Response of Methanol Composition in the Products Using E_m Correlated with $\eta = 0.03$.

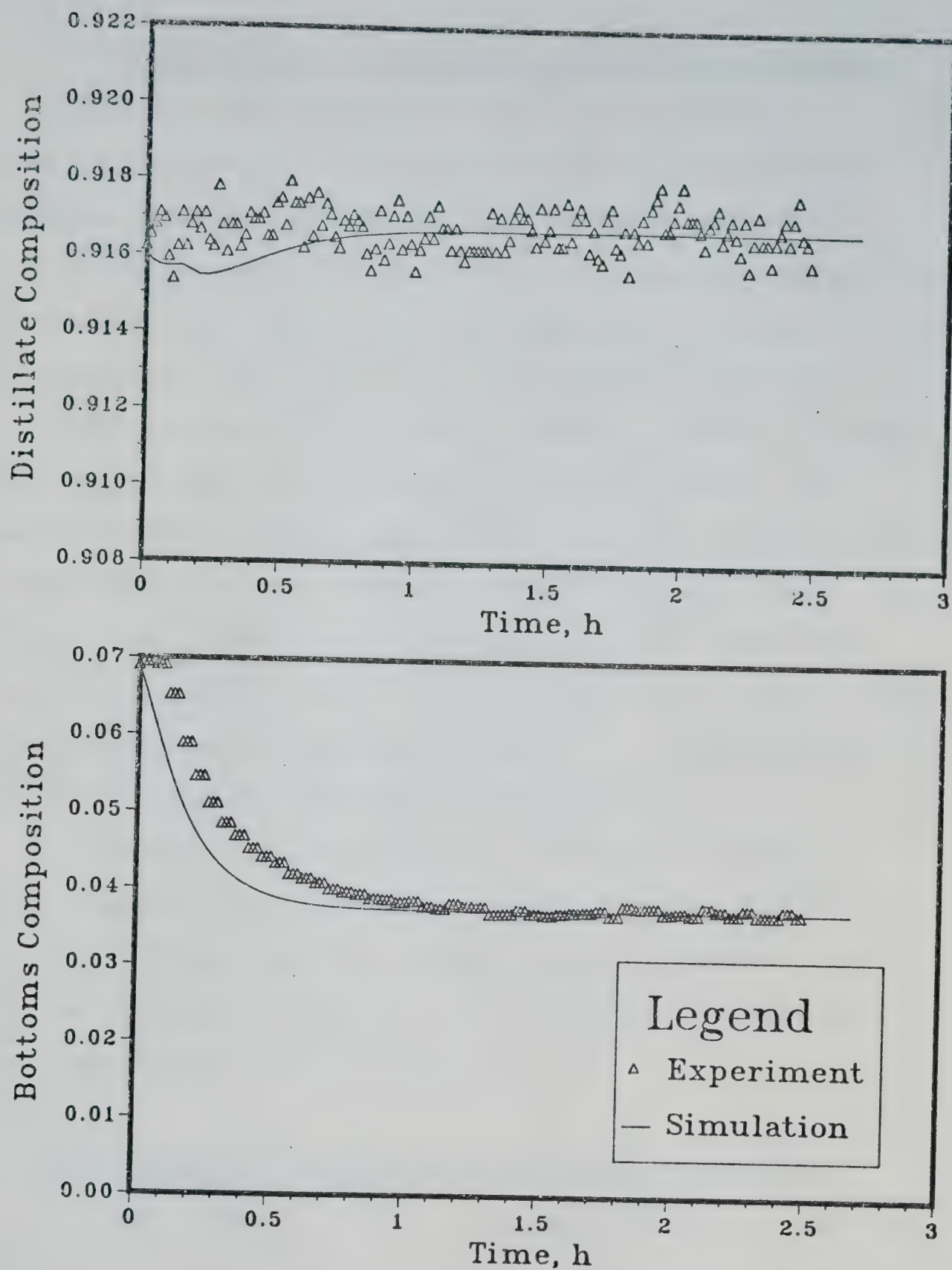


Fig. 5.11 Phase IV Response of Methanol Composition in the Products Using E_m Correlated with $\eta = 0.03$.

6. Simulation of an Extractive Distillation Column

In this chapter the simulation results for an industrial extractive distillation column are presented. The dynamic behavior of the column has been studied by Gallun(13) by simulation using Gear's integration method for systems of stiff equations. The operating conditions for the column can be obtained from Holland and Liapis(12).

The extractive distillation column is controlled using four proportional plus integral (PI) controllers. The feedback control system provides for the regulation of the liquid levels at the condenser and at the base of the column; the condenser pressure and the reflux flow rate. The control system also includes an additional cascade loop, controlling the temperature at stage 35, by manipulation of the amount of steam supplied to the reboiler.

To simulate column behavior, the model in Chapter 2 must therefore be augmented to describe these controllers. In the following sections, changes made to the basic model will be discussed along with the presentation of the open loop and closed loop simulation results.

6.1 Description of the Extractive Distillation Column

In this column, acetone is separated from methanol and ethanol with water as the extractive agent. The column has 48 sieve trays, a reboiler and a total condenser for a total of 50 stages. The tray efficiencies are assumed to be 100% and heat loss to the environment is considered negligible.

The hydraulic parameters used in this simulation are listed in Table 6.1.

Table 6.2
Hydraulic Parameters for the Extractive Distillation Column

Total area of holes	1.208 m ²
Orifice diameter	4.763 mm
Plate thickness	2.381 mm
Effective weir length	3.32 m
Column diameter	4.57 m
Active area of tray	13.13 m ²

There are three feed streams to the column and the feed locations, flow rates and properties are given in Table 6.2. It should be noted that the feed compositions at stage 5 published by Holland and Liapis(12) and Gallun(13) are in error. The compositions in Table 6.2 are correct as indicated by Holland(32) and are consistent with the steady state material balance.

6.2 Simulation of the Initial Steady State

In this simulation, the initial steady state as presented by Holland and Liapis(12) was calculated using the dynamic simulator. The computed steady state is based on a heat input rate of 23.9 MW and a reflux ratio of 2.50. Figure 6.1 is a plot of the computed initial steady state temperature profile as compared to those values reported by

Table 6.2
Properties of Feed Streams

Stage	<u>Component Flow Rate, kmol/h</u>				T_j , K
	methanol	acetone	ethanol	water	
3	0.0	0.0	0.0	136.1	312.5
5	6.80	13.61	136.08	5375.16	342.5
21	1769.04	680.40	136.08	136.08	311.2

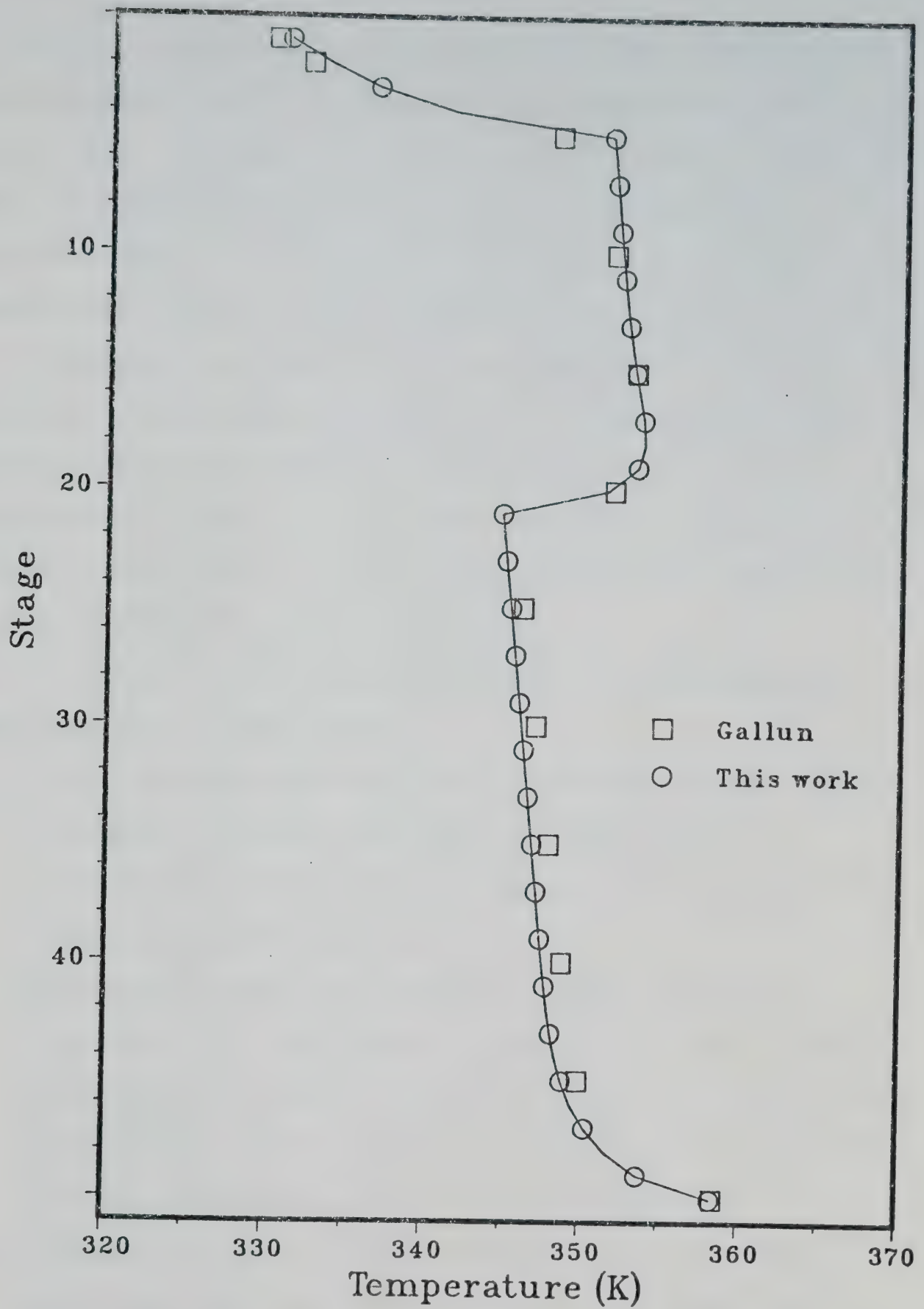


Fig. 6.1: Comparison of Initial Temperature Profiles

Gallun(13). Since Gallun has only given spot values of the stage temperatures, a continuous curve cannot be fitted to the results. However, it can be seen from the plot that the computed temperatures are very close to the published values. Table 6.3 is a partial listing of the initial steady state values of the variables in the column.

Although the computed initial steady state values do not exactly match the published values, the discrepancies are considered to be small enough to justify the use of these values as the initial conditions for the subsequent dynamic simulations. The discrepancies are the result of a number of factors as discussed below.

Firstly is the difference between the thermodynamic models in the following areas:

- i. The parameters for the Wilson equation of state, liquid and vapor enthalpy correlations, molar volume correlation and the Antoine equation are different from those used by Gallun(13).
 - ii. Since the column is operating at about atmospheric pressure, the vapor phase is treated as ideal in this work and the effect of enthalpy departure is neglected. In contrast, Gallun calculated the vapor phase fugacity for the components and the enthalpy departure.
 - iii. Heat of mixing is assumed negligible in this model.
- In these areas the present model uses a more simplified approach. However, the simplifications do not cause much deviation from Gallun's steady state results as can be seen

Table 6.3

Selected Values at the Initial Steady State (GL.SS03)

Stage	Composition in Mole Fraction			
	methanol	acetone	ethanol	water
1	0.0039	0.8102	0.0989	0.0871
2	0.0038	0.6728	0.1623	0.1611
5	0.0019	0.0596	0.0660	0.8725
10	0.0038	0.0594	0.0644	0.8724
15	0.0180	0.0565	0.0519	0.8735
20	0.1091	0.0622	0.0199	0.8087
25	0.2573	0.1183	0.0282	0.5963
30	0.2576	0.1182	0.0282	0.5959
35	0.2580	0.1182	0.0283	0.5955
40	0.2589	0.1174	0.0284	0.5953
45	0.2679	0.1048	0.0294	0.5980
50	0.2302	0.0182	0.0265	0.7251

Stage	P_j , kPa	M_j , kmol	L_j , kmol/s	V_j , kmol/s
1	101.30	127.59	0.475	0.000
2	104.91	11.17	0.450	0.664
5	106.20	35.48	2.004	0.572
10	108.69	35.52	2.006	0.621
15	111.15	35.85	2.010	0.624
20	113.57	35.11	2.038	0.637
25	116.51	35.50	2.846	0.705
30	119.54	35.52	2.851	0.710
35	122.56	35.55	2.856	0.714
40	125.56	35.59	2.860	0.719
45	128.54	35.86	2.859	0.720
50	131.32	1585.30	2.140	0.693

in Figure 6.1 Therefore the more rigorous model of Gallun is not necessary unless the operating pressure is to be increased.

Another factor is the pressure drop correlation employed. In this simulation, the pressure drop across each tray is considered to be due to only two factors:

- i. Dry pressure drop - pressure drop resulting from the entrance loss and frictional loss when the vapor flows through the perforation of the plate, Treybal(28).
- ii. Hydraulic head loss - head loss as a result of the vapor rising through the liquid on the tray, Treybal(28).

Again, the steady state profiles of temperature and pressure obtained from this simulation do not deviate much from those of Gallun, even without the additional terms in Gallun's model. Therefore the two types of pressure drop considered in the present model are sufficient for this column.

The last factor, which does not affect the steady state of the column, is the difference in the tray holdup correlations. The Francis weir formula, Treybal(28), is used in this simulation, whereas Gallun(13) used a modified form of the formula.

6.3 Simulation of the Open-Loop Dynamics

Holland and Liapis(12) have presented the results from a closed loop simulation of the column in which the temperature set point of stage 35 was increased by 2.78 K

from the initial value. However, before performing any closed loop simulations, it is of interest to study the open loop dynamics of the column.

6.3.1 Open Loop Simulation for Step Changes in Reboiler Heat Input

To change the temperature at stage 35 from the initial value to the new set point value, Gallun(13) used the steam flow rate as the manipulated variable. Therefore the simulation of the open loop dynamics in this work also involves step changes in reboiler heat input. The heat input rate is changed by $\pm 10\%$ around the initial value of 23.9 MW. In this simulation the reflux rate is regulated at the initial value of 0.475 kmol/s. The molar holdup at the distillate receiver and at the base of the column are assumed constant, although the tray holdups are variable.

Figures 6.2 and 6.3 show the normalized response of selected stage temperatures for positive and negative changes, respectively. The normalized values are calculated according to the following definition

$$T(\text{normalized}) = \frac{T(t) - T(\text{initial})}{T(\text{final}) - T(\text{initial})} \quad (6.1)$$

The temperature response in Figures 6.2 and 6.3 shows some interesting characteristics. The temperature on stage 20 exhibits inverse behavior for either an increase or decrease in heat input. Upon examination of the inverse response map

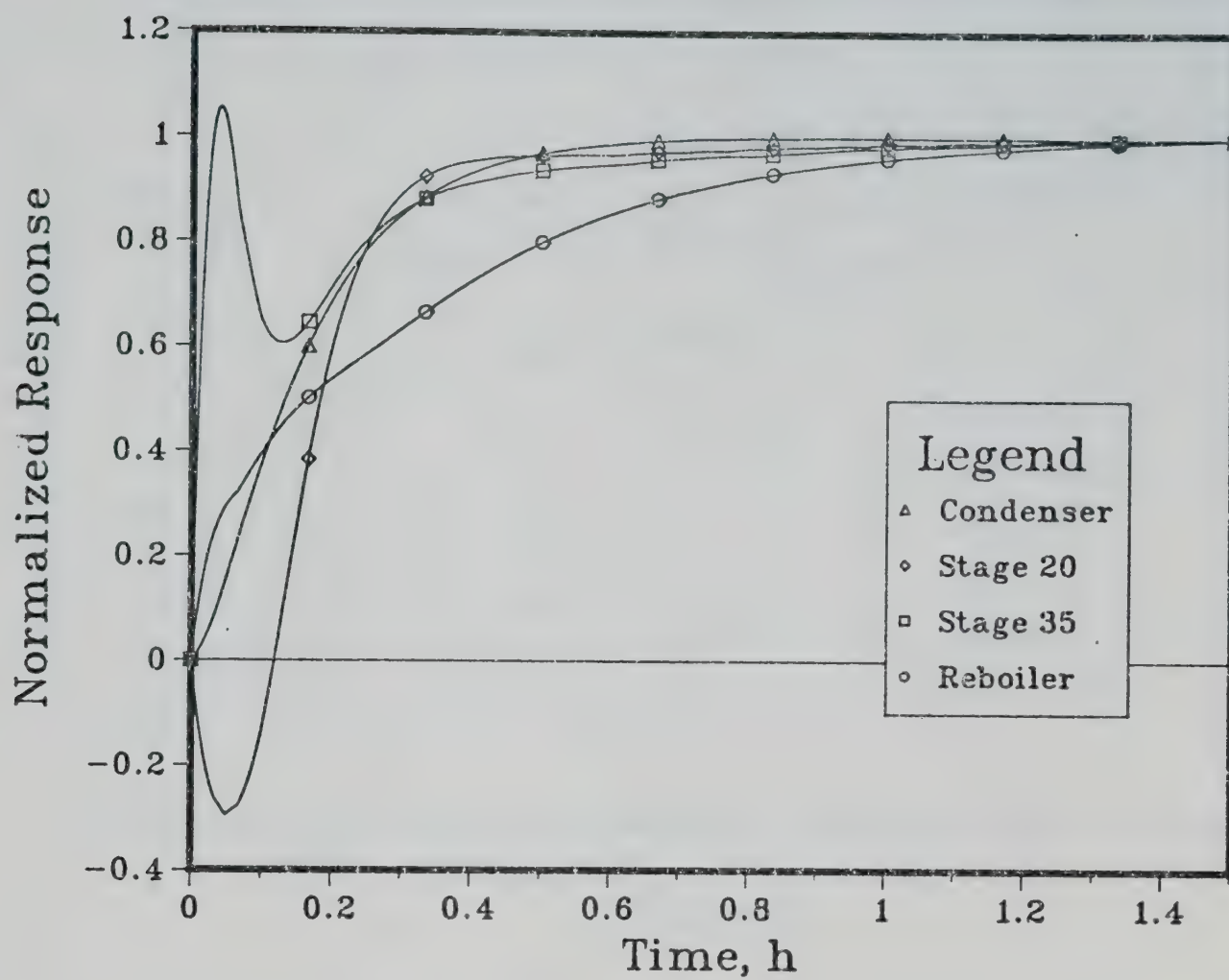


Fig. 6.2 Open Loop Temperature Response for +10% step change in Q_r (Test: GL.QR.OL15)

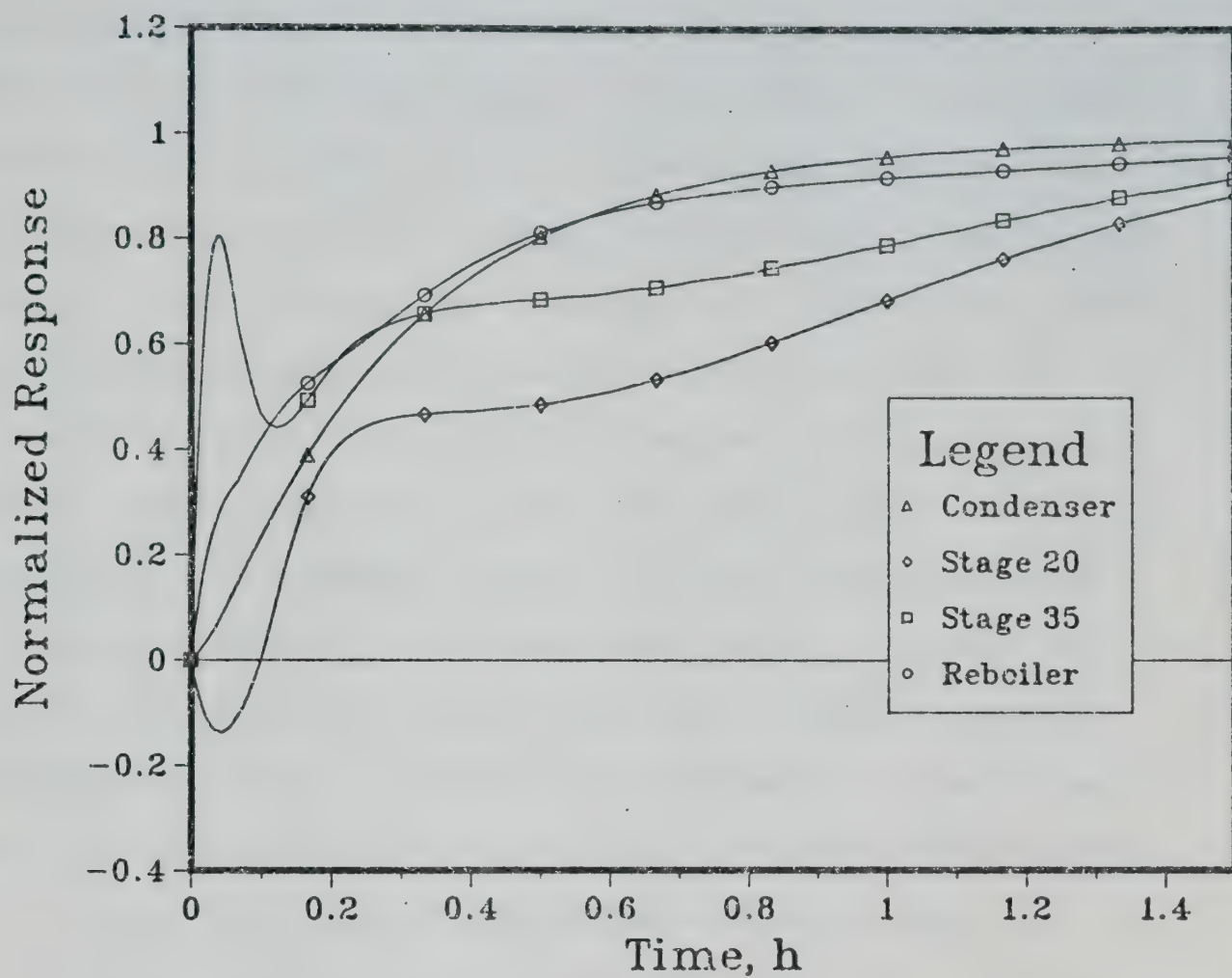


Fig. 6.3 Open Loop Temperature Response for -10% step change in Q_r (Test: GL.QR.OL16)

in Table 6.4, it can be seen that stage 20 is the only stage in which inverse response in temperature occurs.

The temperature response on stage 35 is also interesting since the temperature changes abruptly immediately after the change in heat input. This change is caused by the sudden change in the column pressure which has an immediate effect on the equilibrium temperature on the stage. After this initial change, the temperature follows an inverse pattern very similar to that on stage 20. However because of the initial change, the change to the final steady state is in the same direction as the initial change so the response cannot be classified as inverse response. However this nonminimum phase characteristic can still degrade control performance and causes excessive response overshoot, as will be discussed in a later section dealing with servo control using a cascade control system.

From the inverse response map given as Table 6.4, it is also found that methanol, component 1, exhibits inverse response behavior in the bottoms product for the increase in heat input. Therefore, unlike the results in Chapter 4, for this column one species has exhibited inverse behavior even when it is present as an impurity in the product streams.

It can also be seen that the dynamics of the stage temperature is slower for a decrease in heat input. The temperatures at the intermediate stages are especially slow to respond, not having reached a steady state after 1.5 hours of simulation time.

Table 6.4: Inverse Response Map for Heat Input Changes

+10% change (GL.QR.OL15)

-10% change (GL.QR.OL16)

STAGE	TEMP	COMPONENT			
		1	2	3	4
1	.	.	.	.	.
2	.	.	.	.	.
3	.	.	.	.	.
4	.	.	.	*	.
5	.	.	.	.	.
6	.	.	.	.	.
7	.	.	.	.	.
8	.	.	.	.	.
9	.	.	.	.	.
10	.	.	.	.	.
11	.	.	.	.	.
12	.	.	.	.	.
13	.	.	.	.	.
14	.	.	.	.	.
15	.	.	.	.	.
16	.	.	.	.	.
17	.	.	.	.	*
18	.	.	.	.	*
19	.	.	.	.	*
20	T	.	*	.	.
21	.	.	*	.	.
22	.	.	*	.	.
23	.	.	*	.	.
24	.	.	*	.	.
25	.	.	*	.	.
26	.	.	*	.	.
27	.	.	*	.	.
28	.	.	*	.	.
29	.	.	*	.	.
30	.	.	*	*	.
31	.	.	*	.	.
32	.	.	.	.	.
33	.	.	.	.	.
34	.	.	.	.	.
35	.	.	.	.	*
36	.	.	.	*	.
37	.	.	.	*	*
38	.	.	.	*	.
39	.	.	.	.	.
40	.	.	.	*	.
41	.	.	.	*	.
42	.	.	.	*	.
43	.	.	.	*	.
44	.	.	.	*	.
45	.	.	.	*	.
46	.	.	.	*	.
47	.	.	.	*	.
48	.	.	.	*	.
49	.	.	.	*	.
50	.	*	.	.	.

STAGE	TEMP	COMPONENT			
		1	2	3	4
1	.	.	.	.	.
2	.	.	.	.	.
3	.	.	.	.	.
4	.	.	.	.	.
5	.	.	.	*	.
6	.	.	.	*	.
7	.	.	.	*	.
8	.	.	.	*	.
9	.	.	.	*	.
10	.	.	.	*	.
11	.	.	.	*	.
12	.	.	.	*	.
13	.	.	.	*	.
14	.	.	.	*	.
15	.	.	.	.	.
16	.	.	.	.	.
17	.	.	.	.	*
18	.	.	.	.	*
19	.	.	.	.	*
20	T	.	*	.	.
21	.	.	*	.	*
22	.	.	*	.	*
23	.	.	*	.	*
24	.	.	*	.	*
25	.	.	*	.	*
26	.	.	*	.	*
27	.	.	*	.	*
28	.	.	*	.	*
29	.	.	*	.	*
30	.	.	*	.	*
31	.	.	.	*	*
32	.	.	.	*	*
33	.	.	.	*	*
34	.	.	.	*	*
35	.	.	.	*	*
36	.	.	.	*	.
37	.	.	.	.	.
38	.	.	.	.	*
39	.	.	.	*	.
40	.	.	.	*	.
41	.	.	.	.	.
42	.	.	.	*	.
43	.	.	.	*	.
44	.	.	.	*	.
45	.	.	.	*	.
46	.	.	.	*	.
47	.	.	.	*	.
48	.	.	.	*	.
49	.	.	.	*	.
50	.	*	.	.	.

* - COMPOSITION INVERSE RESPONSE
T - TEMPERATURE INVERSE RESPONSE
. - NORMAL RESPONSE

Figure 6.4 and Figure 6.5 are the composition profiles of acetone and methanol, respectively, for the initial and final steady states.

6.4 Closed Loop Simulation for Step Changes in Reboiler Heat Input

In the open loop simulation as discussed previously, the column is simulated with a constant molar holdup at both the distillate receiver and the column base. The assumption of constant holdup in these locations has the effect that the response of the product flow rates to any change in heat input is almost immediate since the overhead receiver and the column base do not provide any damping for the flow rates. In a typical industrial column, however, the liquid levels at the distillate receiver and at the column base are often regulated by automatic controllers which inevitably introduce dynamics to the molar holdups. In this section, the modelling equations are discussed and the damping effects on the response of the product flow rates are illustrated by computer simulations.

6.4.1 Modelling of Liquid level Controllers

At the top of the column two control loops are regulating the overhead receiver liquid level and the reflux flow rate respectively. To model these controllers the following equations are written

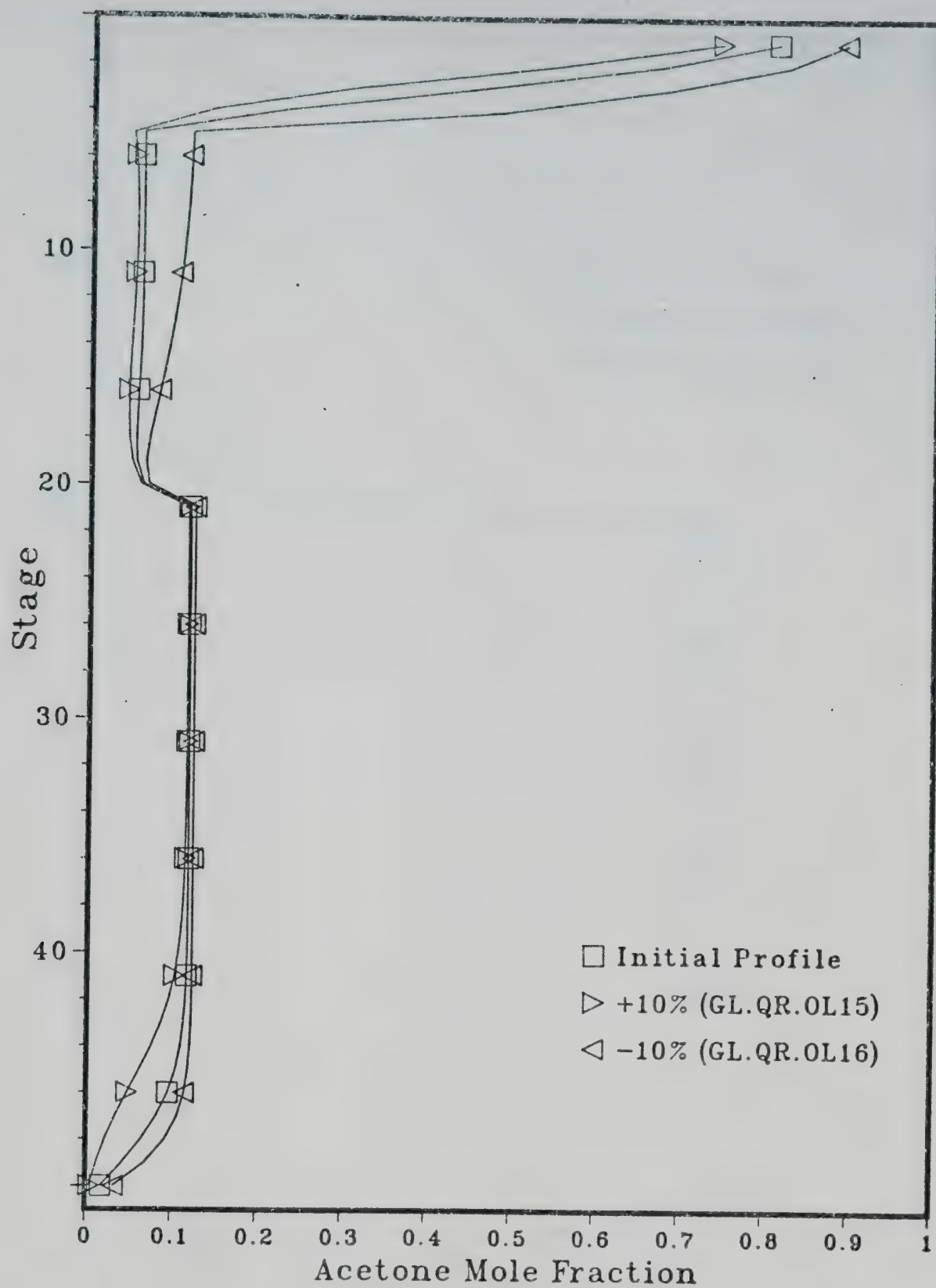


Fig. 6.4: Steady State Composition Profiles of Acetone for Heat Input Changes

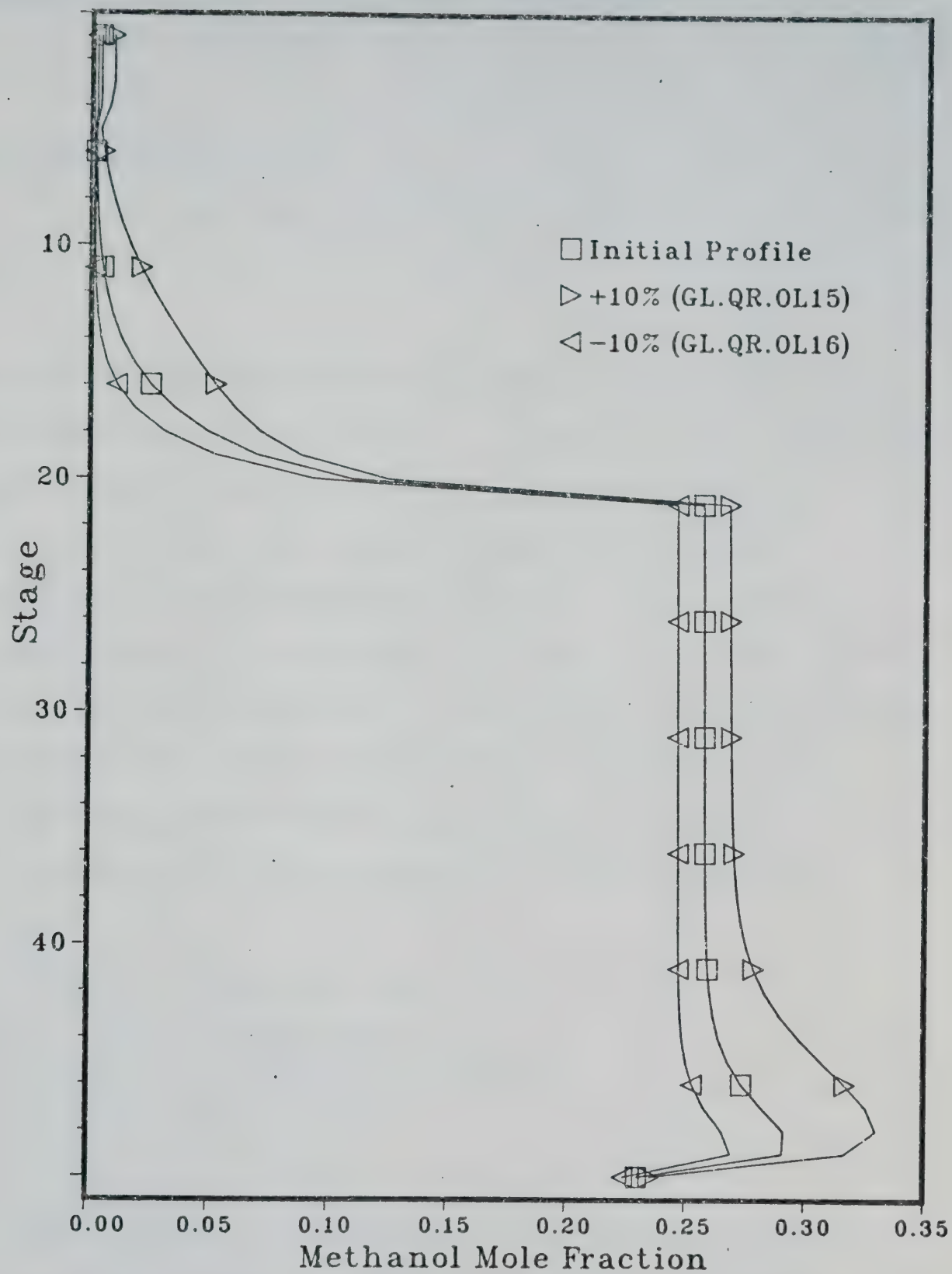


Fig. 6.5: Steady State Composition Profiles of Methanol for Heat Input Changes

Distillate Receiver Liquid Level Controller:

$$D = Kp_3 (z_1 - z_1'') + D' \quad (6.2)$$

Reflux Flow Controller:

$$L_1 = Kp_2 (e_2 + Ki_2 \int_0^t e_2 dt) + L_1' \quad (6.3)$$

where $e_2 = L_1'' - L_1$

The controller constants are subscripted according to the loop number used by Gallun(13). However, in this study, the liquid level is controlled using only a proportional controller rather than a proportional plus integral controller as used by Gallun. Integral action was not employed since it is generally not desirable to have perfect control on the liquid level as the receiver holdup should be allowed to float to absorb the effects of disturbances.

By making use of equations 6.2 and 6.3, the following two ordinary differential equations can be established

$$\frac{d}{dt} \begin{bmatrix} M_1 \\ L_1 \end{bmatrix} = \begin{bmatrix} V_2 - L_1 + Kp_3(z_1'' - z_1) - D' \\ \frac{(Kp_2)(Ki_2)}{(1+Kp_2)} (L_1'' - L_1) \end{bmatrix} \quad (6.4)$$

The first equation is obtained by substituting equation 6.1 into the mass balance equation for the receiver holdup

$$(dM_1/dt) = V_2 - L_1 - D \quad (6.5)$$

while the second equation results from differentiating equation 6.3 with respect to time.

Assuming that the receiver liquid level is some function of the molar holdup

$$z_1 = g\{M_1\} \quad (6.6)$$

allows the Jacobian of equation 6.3 to be written as

$$\underline{J} = \begin{bmatrix} -Kp_3 \frac{\partial g}{\partial M_1} & -1 \\ 0 & \frac{-Ki_2}{1+Kp_2} \end{bmatrix} \quad (6.7)$$

Appending this Jacobian matrix to the top of the Jacobian corresponding to the tray hydraulics (cf. equation 2.17) does not destroy the tridiagonal structure so the holdup, M_1 , and liquid flow rate, L_1 , can be solved along with the liquid flow rates using the normal integration scheme.

The required steps to include the liquid level controller at the base of the column are similar to those required to include the receiver liquid level controller. The proportional controller can be described as

$$L_n = Kp_5 (z_n - z_n'') + L_n' \quad (6.8)$$

so the mass balance for the liquid phase at the column base

can be expressed as

$$(dM_n/dt) = L_{n-1} - V_n - Kp_5(z_n - z_n'') - L_n \quad (6.9)$$

Equation 6.8 forms another equation which can be solved simultaneously with the liquid flow rates. The equation introduces two additional elements to form the last row of the Jacobian matrix corresponding to the tray hydraulics

$$\partial \dot{M}_n / \partial L_{n-1} = 1 \quad \text{and} \quad (6.10)$$

$$\partial \dot{M}_n / \partial M_n = -Kp_5 [dg/dM_n] \quad (6.11)$$

again assuming the functional relationship between liquid level and molar holdup. The tridiagonal structure of the Jacobian matrix remains unaltered.

For the regulation of the condenser pressure, it is assumed that the pressure controller is capable of perfect control such that any deviation of the condenser pressure from the set point value is negligible.

6.4.2 Closed Loop Simulation Results

In the closed loop simulation of the response of the column to heat input changes, the liquid level controllers and the reflux flow controller modelled previously are used to provide regulatory actions against the disturbance. The

controller parameters used are taken as those used by Gallun(13). However, since the liquid level controllers modelled in this work are proportional controllers only, the reset times used by Gallun are not applicable.

As in the open loop simulation, the heat input is changed by $\pm 10\%$ from the initial value of 23.9 MW in this simulation. The response of the product flow rates are plotted in Figures 6.6 and 6.7. As can be seen, the dynamic behavior of the product flow rates with and without the controllers are quite different. The dynamics provided by the liquid level controllers tends to slow down the abrupt change in the product flow rates caused by the disturbance. However, the dynamics of the stage temperatures is not altered significantly from the open loop dynamics by the controllers as seen in Figures 6.8 and 6.9.

6.5 Closed-Loop Simulation for Temperature Set Point Change

6.5.1 Modelling of a Cascade Proportional Plus Integral Control Loop

The results from the open loop simulation clearly indicate that it is feasible to control the stage temperature via the manipulation of heat input. In this closed loop simulation the temperature at stage 35 is controlled by a cascade controller similar to the arrangement used by Gallun(13).

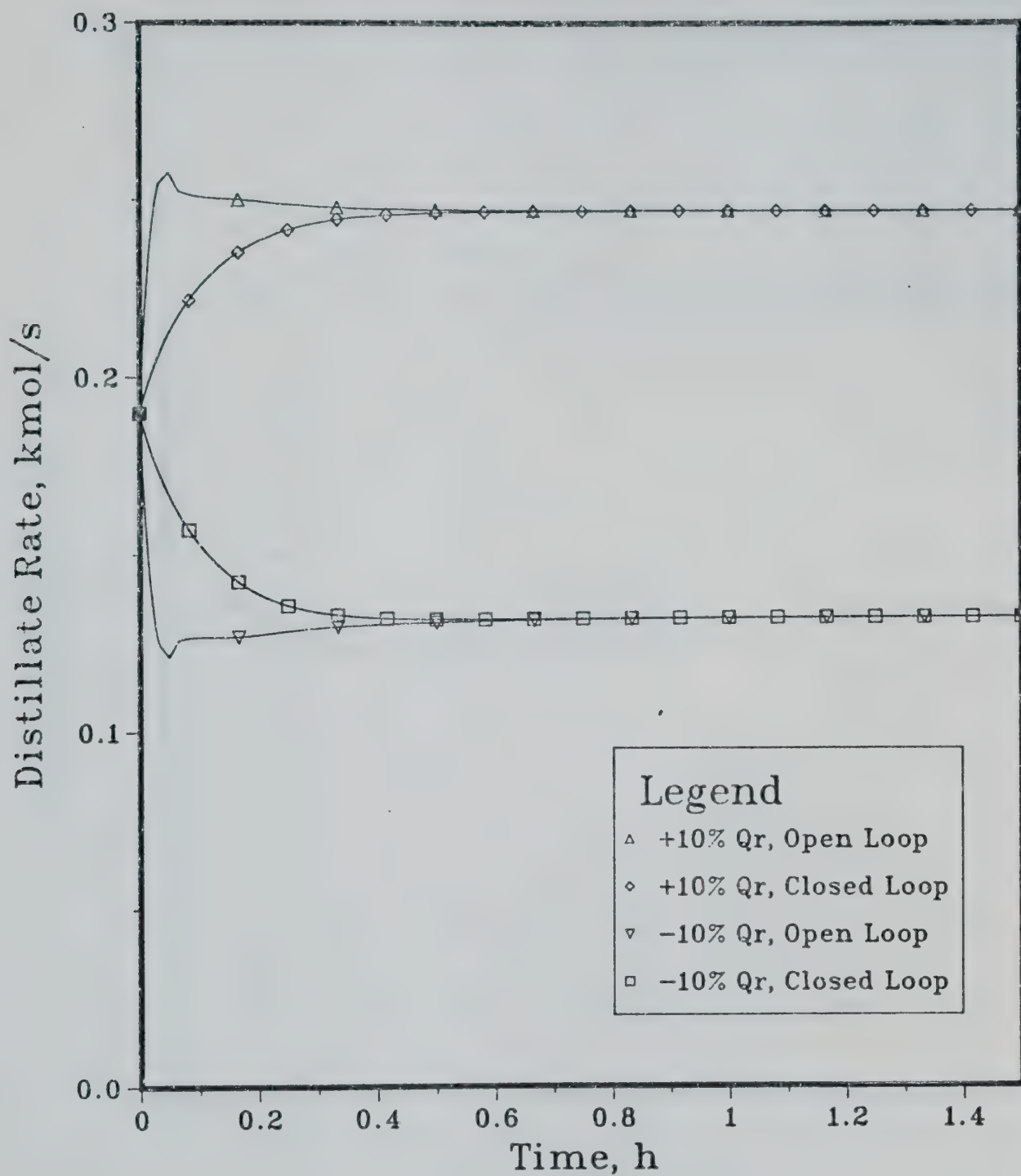


Fig. 6.6: Comparison of Open Loop and Closed Loop Distillate Flow Rate

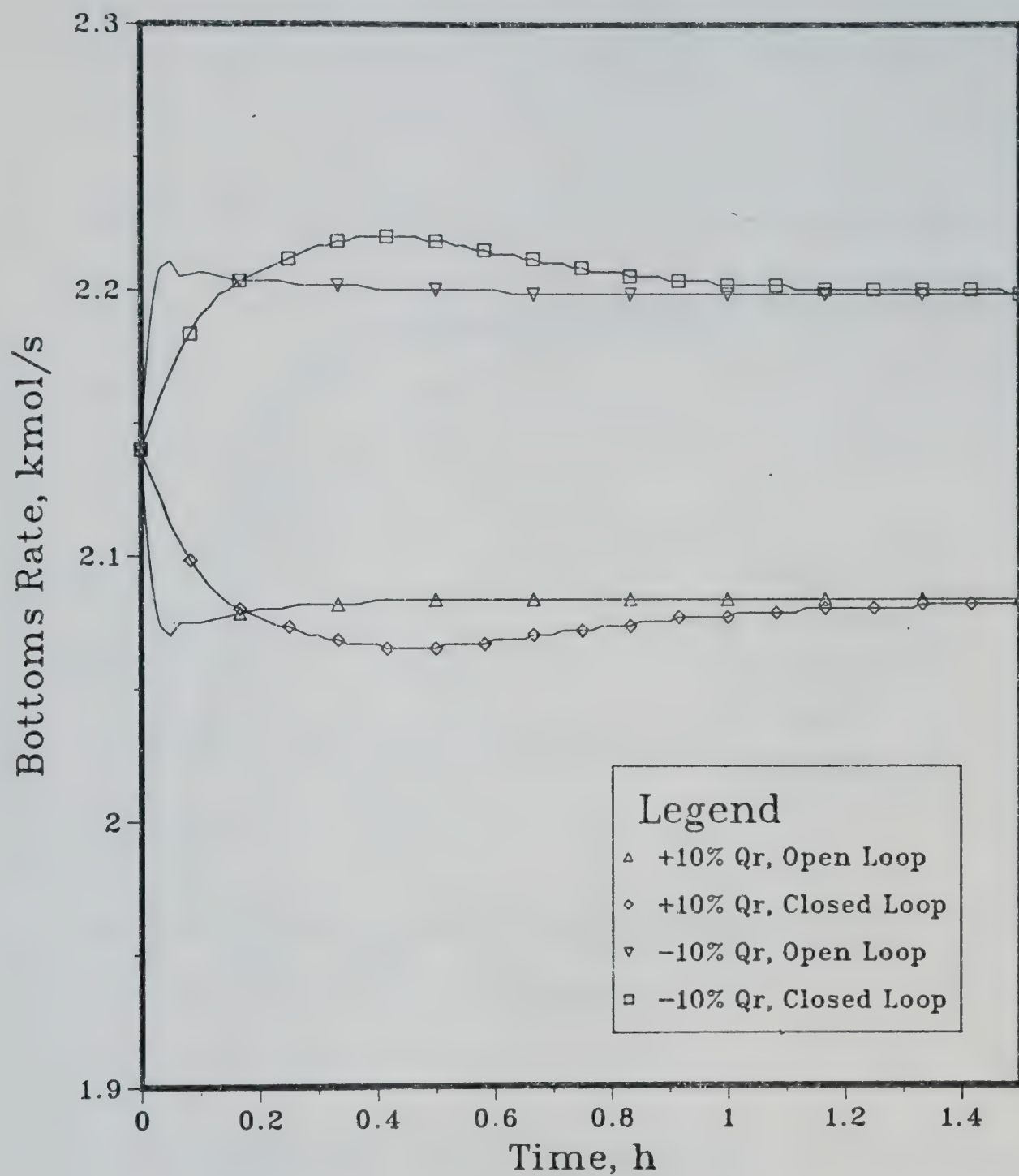


Fig. 6.7: Comparison of Open Loop and Closed Loop Bottoms Flow Rate

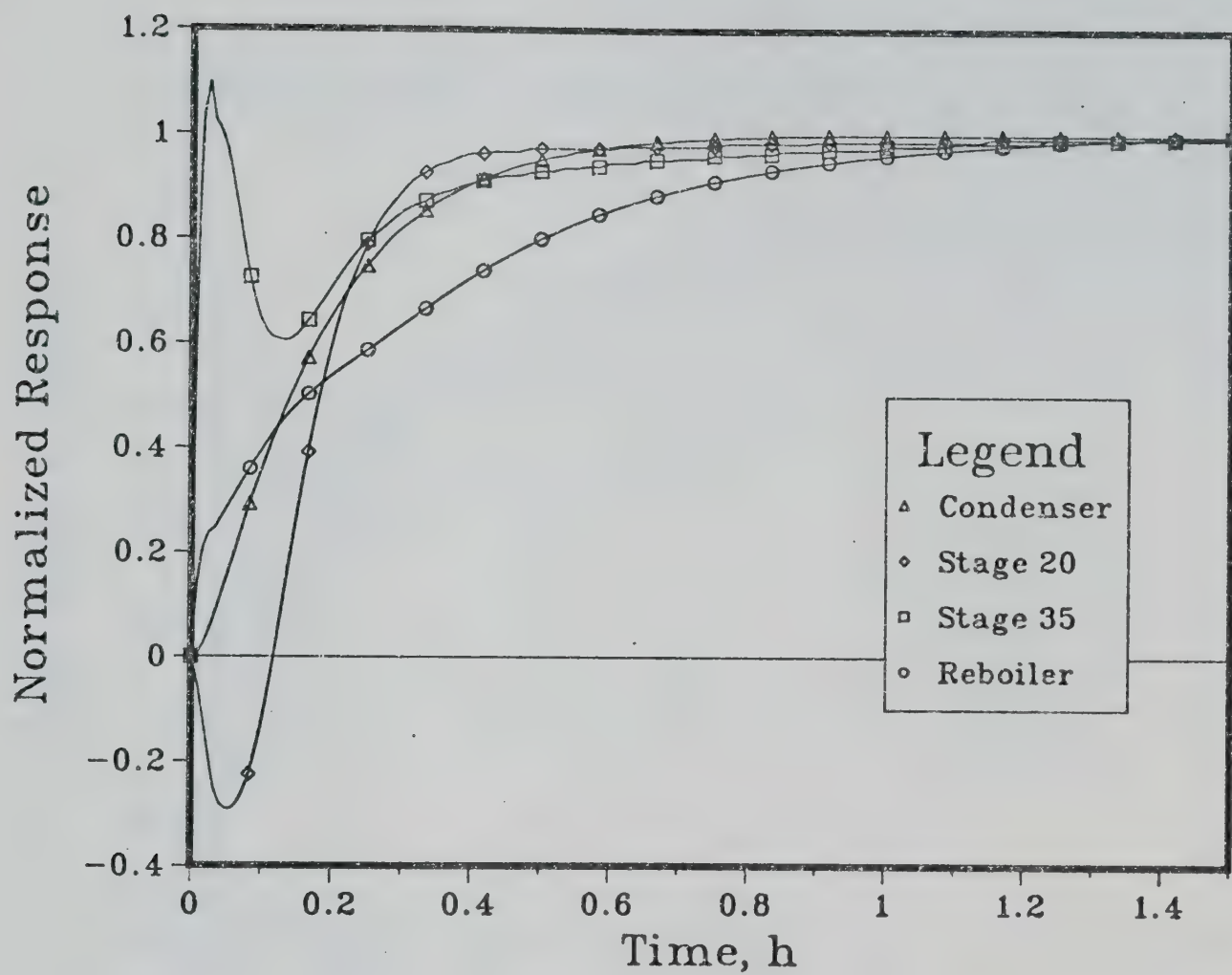


Fig. 6.8 Closed Loop Temperature Response for +10% step change in Q_r (Test: GL.QR.OL13)

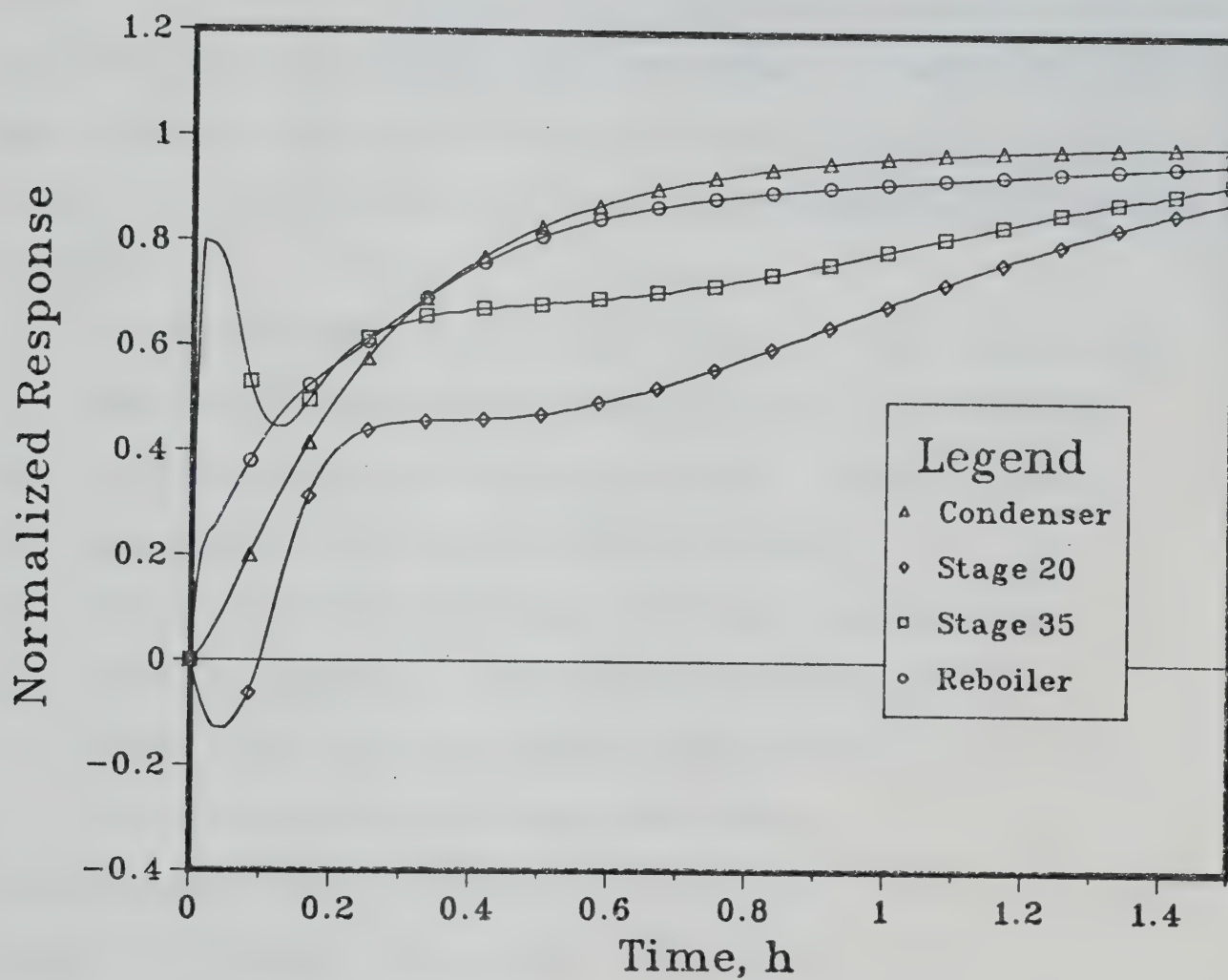


Fig. 6.9 Closed Loop Temperature Response for -10% step change in Q_r (Test: GL.QR.OL14)

For the column studied by Gallun, the proportional plus integral master loop (PI) controls the temperature at stage 35 and produces a set point for the slave steam flow controller, which is a PI flow controller.

In this simulation the controllers are also arranged in a cascade manner. However, unlike the study of Gallun, the column simulation has been performed with the master control loop being a discrete data PI controller, although the slave loop remains to be a continuous PI steam flow controller. In modelling such control system, the following assumptions are made

- i. the dynamics of the control valve and the temperature measurement device are considered to be negligible;
- ii. the computation of the new control action is fast compared to the sample time interval;
- iii. the rate of heat transfer from the steam to the reboiler liquid is instantaneous and that it is possible to directly measure and manipulate the heat flux instead of the steam flow rate.

The consequence of assumption (i) and (ii) is that the delay between the sample measurement and control action is negligible. Assumption (i) also simplifies the calculations since the modelling equations for the control valve and the measurement device become algebraic. Assumption (iii) is used to eliminate the need to account for the dynamics resulting from heat transfer. The validity of the assumption is uncertain, but Gallun did not consider the

dynamics of the reboiler, so the same approach is followed in this work.

On the basis of these assumptions the following equations are written to describe the control system. For the discrete master control loop:

$$c_6^k = 0.72(T_{35}^k) - 236 \quad (6.12)$$

$$r_6^k = 0.72(T_{35}^k) - 236 \quad (6.13)$$

$$e_6^k = r_6^k - c_6^k \quad (6.14)$$

$$I_6^k = \sum_i [(e_6^k + e_6^{k-1}) T_s / 2] \quad i=0, 1, \dots, k \quad (6.15)$$

$$p_6^k = Kp_6[e_6^k + I_6^k/\tau_6] + p_6^i \quad (6.16)$$

Equation 6.12 converts the measured temperature in Kelvin to a value between 4 to 20, ie. the range of measurement is between 333.33 K to 355.56 K. Similar conversion is applied to the temperature set point in equation 6.13 and the error is computed with equation 6.14. The error integral of the master loop in equation 6.15, in which T_s represents the sample interval, is calculated by trapazoidal integration rule. The output signal from the master is calculated in equation 6.16 using a proportional plus integral algorithm.

For the slave loop regulating the steam flow rate to the reboiler, the following equations are written:

$$c_4 = 0.005017(Q_r) + 4 \quad (6.17)$$

$$e_4 = p_6^k - c_4 \quad (6.18)$$

$$I_4 = \int_0^t e_4 \, dt \quad (6.19)$$

$$p_4 = Kp_4[e_4 + I_4/\tau_4] + p_4^i \quad (6.20)$$

$$Q_r = 199.34(p_4) - 797.35 \quad (6.21)$$

The current heat input rate is converted to a value between 4 and 20 in equation 6.17. In this equation the heat input rate is in MJ/min, and the equivalent maximum rate is 53.16 MW, which corresponds to the maximum steam input rate of 3,000 lb/min given by Gallun(13). Equation 6.18 defines the error for the slave controller and the error integral is obtained in equation 6.19. The output signal from the slave controller is calculated in equation 6.20 to give a value between 4 to 20. Finally the heat input rate is converted from the output signal in equation 6.21 to a heat flux unit in MJ/min.

Based on equations 6.17 to 6.21, the heat input rate can be described as

$$\frac{dQ_r}{dt} = \left[\frac{Kp_4}{1 + Kp_4} \right] \left[\frac{1}{0.005017 \, \tau_4} \right] [e_4] \quad (6.22)$$

To solve for Q_r , one may write the Jacobian of equation 6.22 as

$$\frac{\partial \dot{Q}_r}{\partial Q_r} = \left(\frac{-Kp_4}{1 + Kp_4} \right) \left(\frac{1}{\tau_4} \right) \quad (6.23)$$

It may be interesting to note that in this single feedback

control loop, the Jacobian reduces to a scalar. Equations 6.22 and 6.23 can be used in the ASIRK method to solve for the value of Q_r .

In the modelling of this cascade control system, it is assumed that the initial values of the errors and the error integrals are zero. The initial value of the measured value and the heat input rate are equal to their initial steady state values. The temperature set point is changed to the new value at time 0⁻ of the simulation.

6.5.2 Closed Loop Simulation Results

In this simulation the temperature set point of stage 35 is increased or decreased from the initial value of 346.81 K. The controller parameters for the cascade loop given by Gallun(13) are used in an initial test and the master loop sample interval set to 6 seconds for a total simulation time of 5400 seconds. Using the controller parameters given by Gallun, which are

$$Kp_6 = 0.50$$

$$\tau_6 = 0.60 \text{ min.}$$

$$Kp_4 = 0.15$$

$$\tau_4 = 0.25 \text{ min.}$$

the column response to a step change in the temperature set point to 349.59 K is simulated. As seen from Figure 6.10, the temperature response has a significantly higher overshoot than the published response, and is more oscillatory. This simulation test, performed on an FPS-164

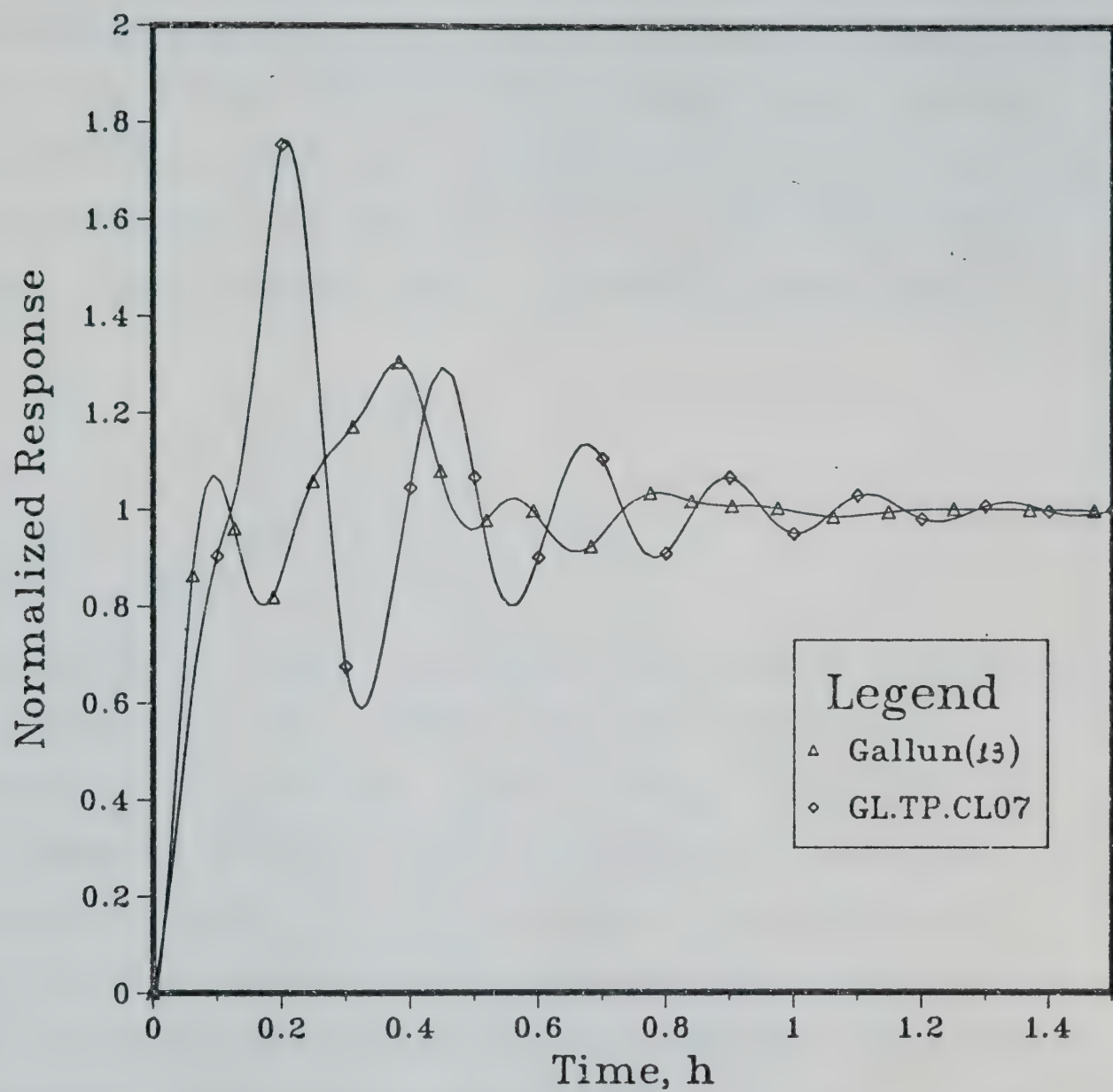


Fig. 6.10: Comparison of the Temperature Response on Stage 35 to Decrease in Temperature Set Point

Attached Processor, required 945.3 seconds to complete.

Several different sets of controller parameters, other than the ones given by Gallun(13), have been used in the simulation studies in an effort to improve the closed loop behavior. It was found that the response can be improved significantly merely by increasing the proportional gains in both the master loop and the slave loop using the original value of the integral times. For example, using parameters of

$$Kp_6 = 0.80$$

$$\tau_6 = 0.60 \text{ min.}$$

$$Kp_4 = 0.30$$

$$\tau_4 = 0.25 \text{ min.}$$

provide better control performance, as shown by the results in Figure 6.11. The response characteristics of the simulation using Gallun's parameter value (GL.TP.CL07) and the response using the improved parameters (GL.TP.CL08) are compared in Table 6.5. The response of the manipulated variable for the two tests is also plotted in Figure 6.12. To illustrate the response of other variables, the product flow rates, the ethanol composition in the distillate and the acetone composition in the bottom product are plotted in Figures 6.13, 6.14, 6.15 and 6.16, respectively.

Although the closed loop performance can be improved by increasing the proportional gains for an increase in set point, this is not the case for a decrease in set point. This behavior arises because at the initial steady state,

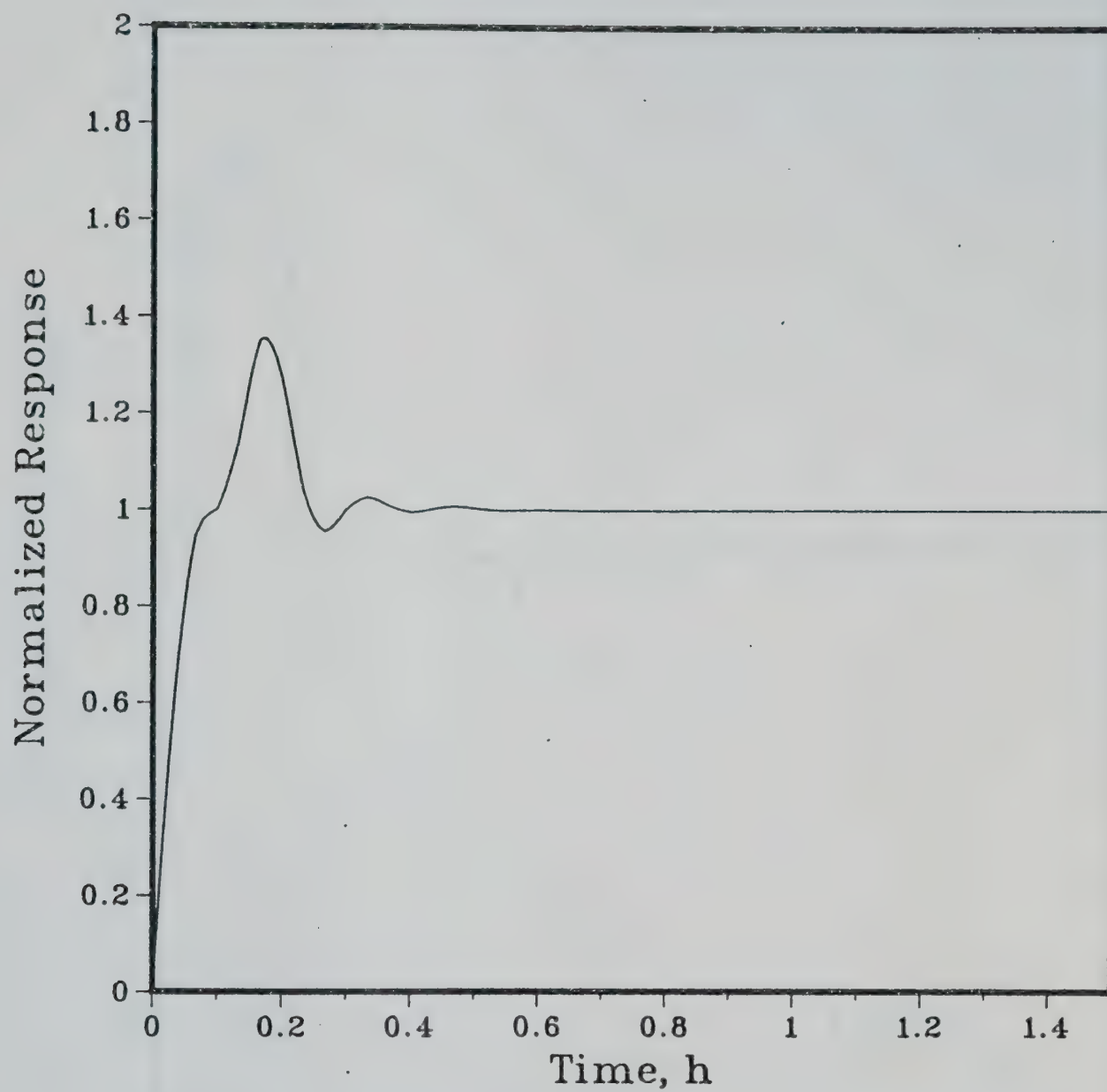


Fig. 6.11: Temperature Response on Stage 35
using Improved Controller Parameters

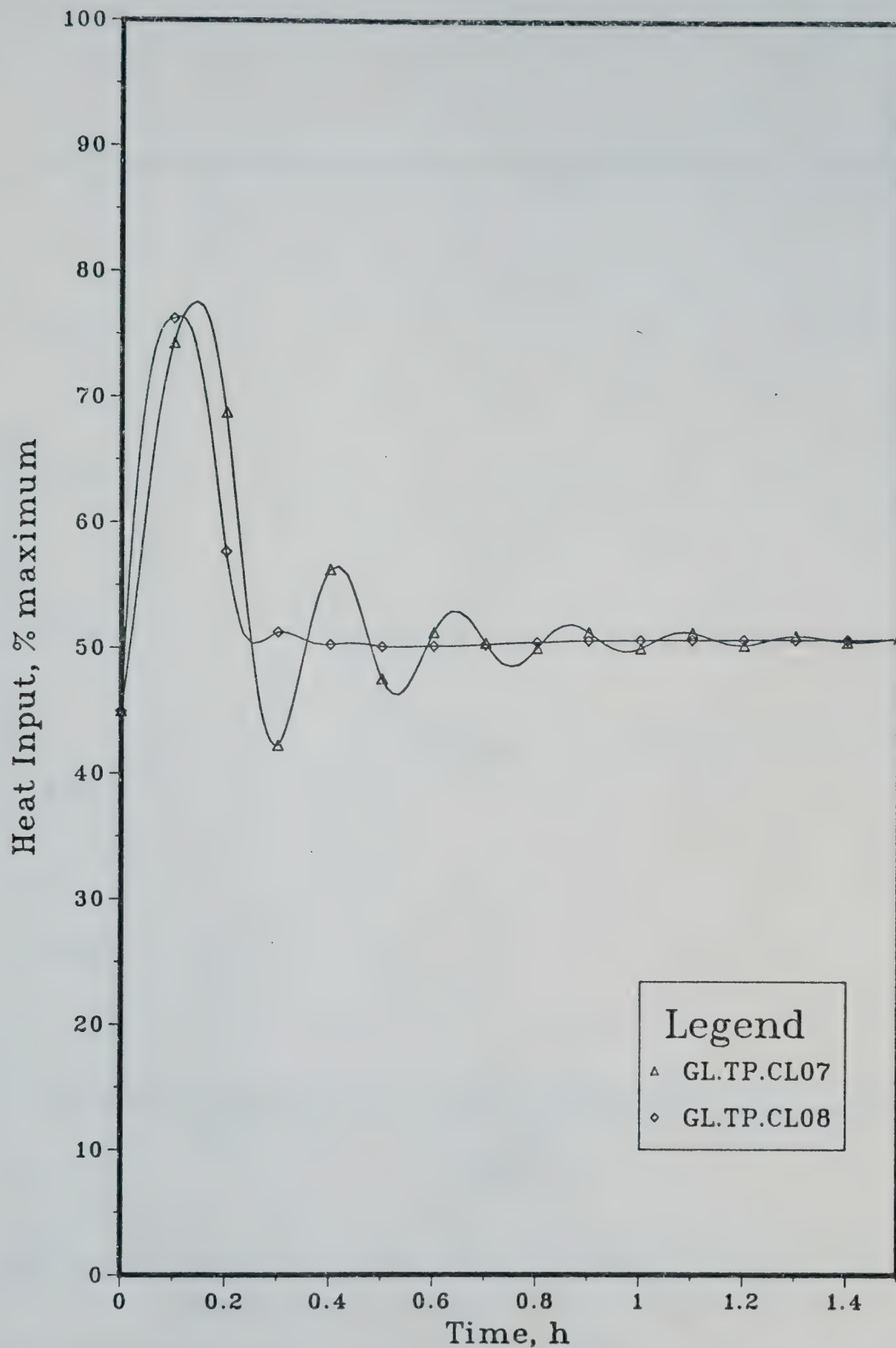


Fig. 6.12: Comparison of Heat Input Response to Decrease in Temperature Set Point

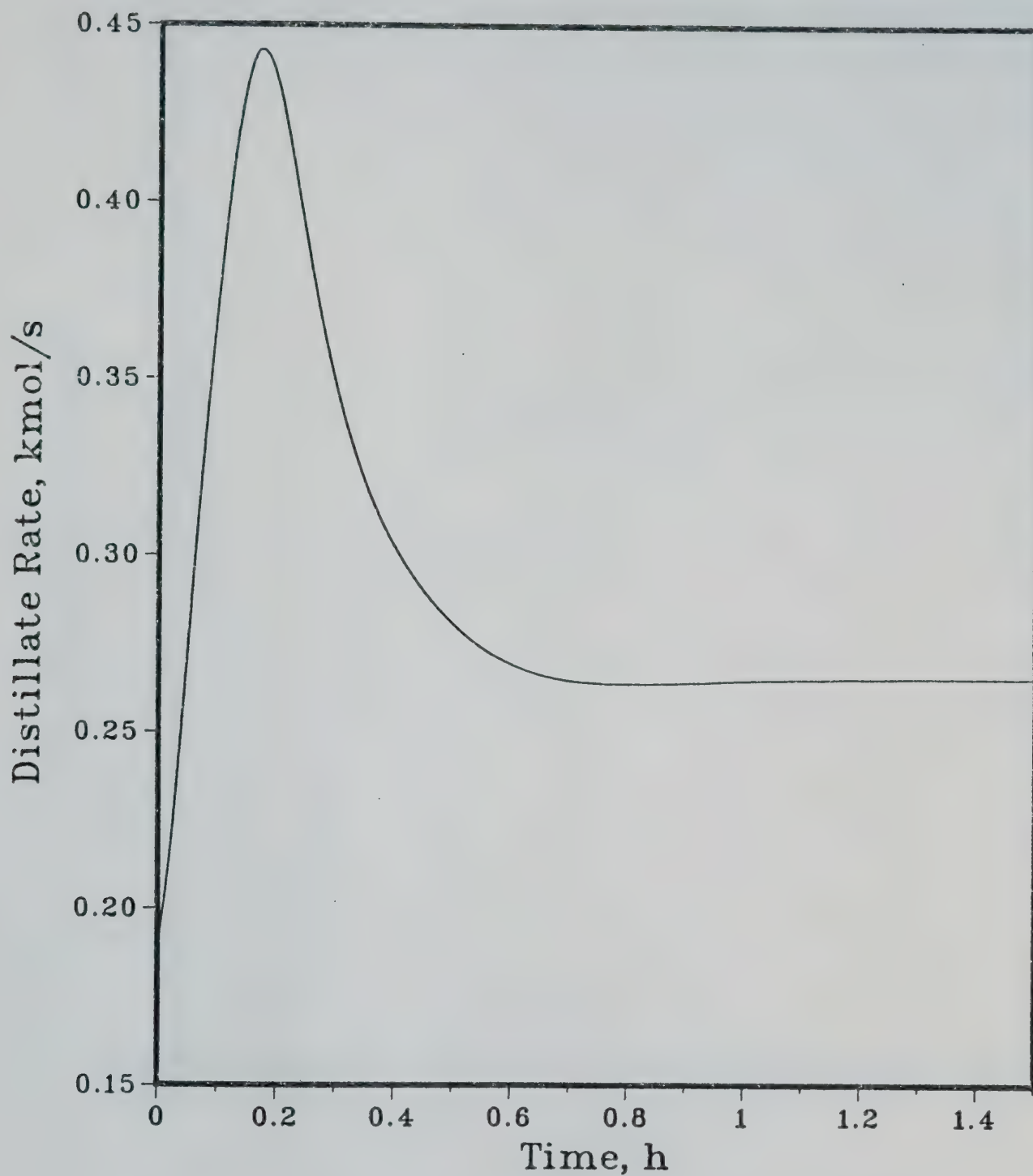


Fig. 6.13: Response of Distillate Flow Rate to Decrease in Temperature Set Point

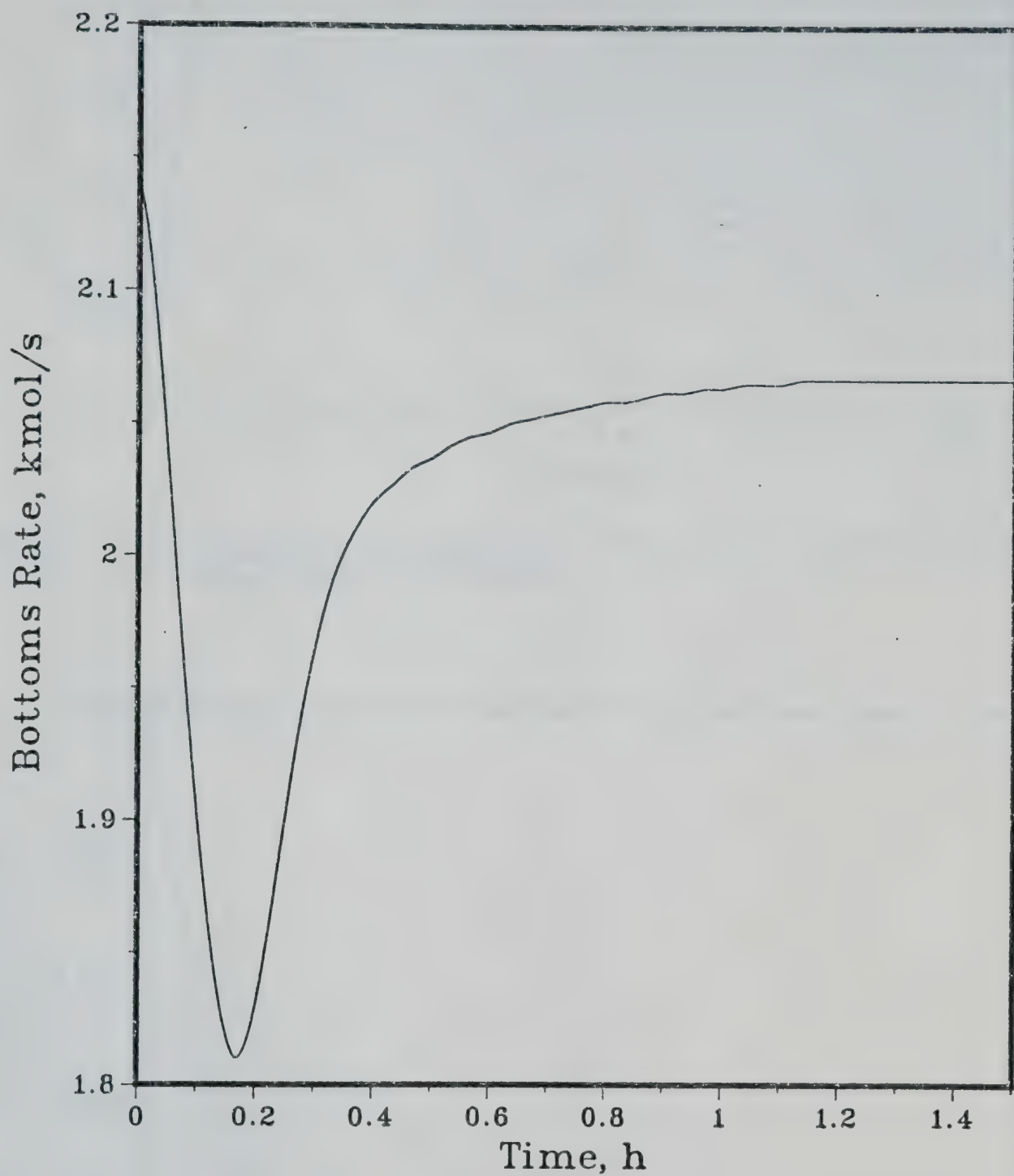


Fig. 6.14: Response of Bottoms Flow Rate to Decrease in Temperature Set Point

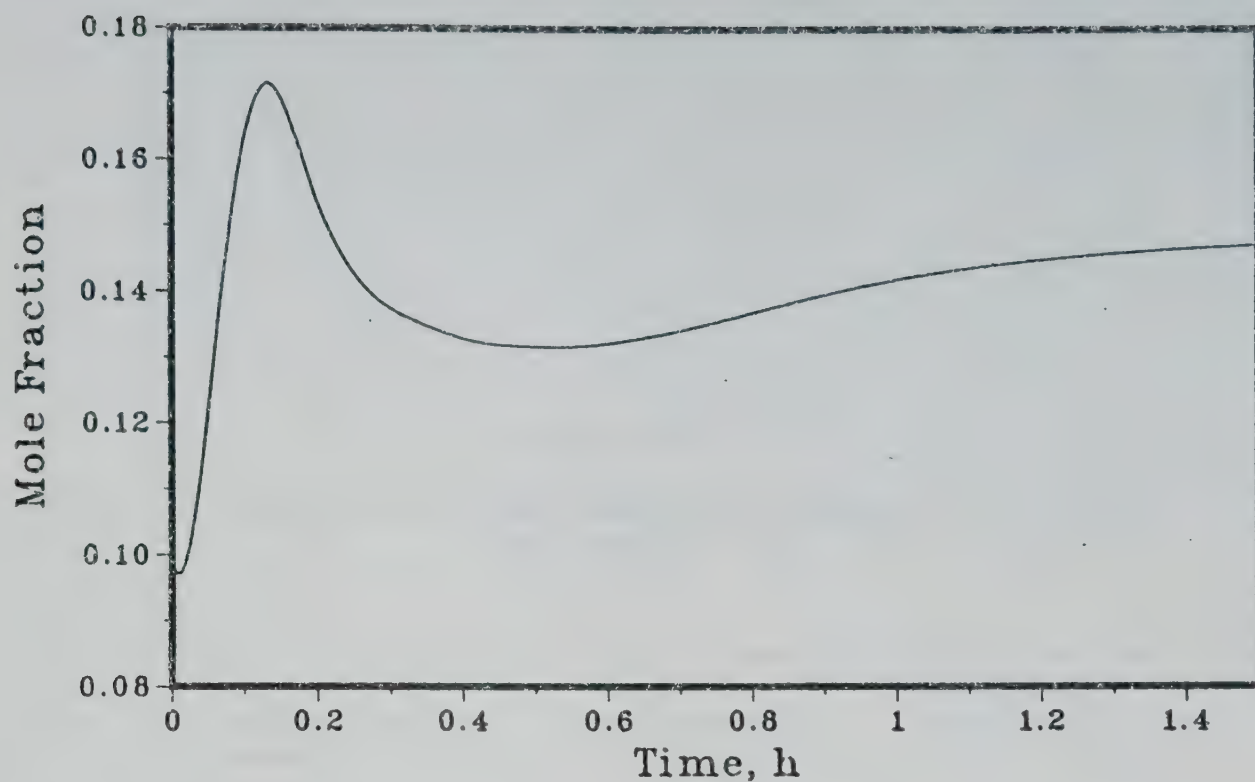


Fig. 6.15: Response of Ethanol in Distillate to Decrease in Temperature Set Point

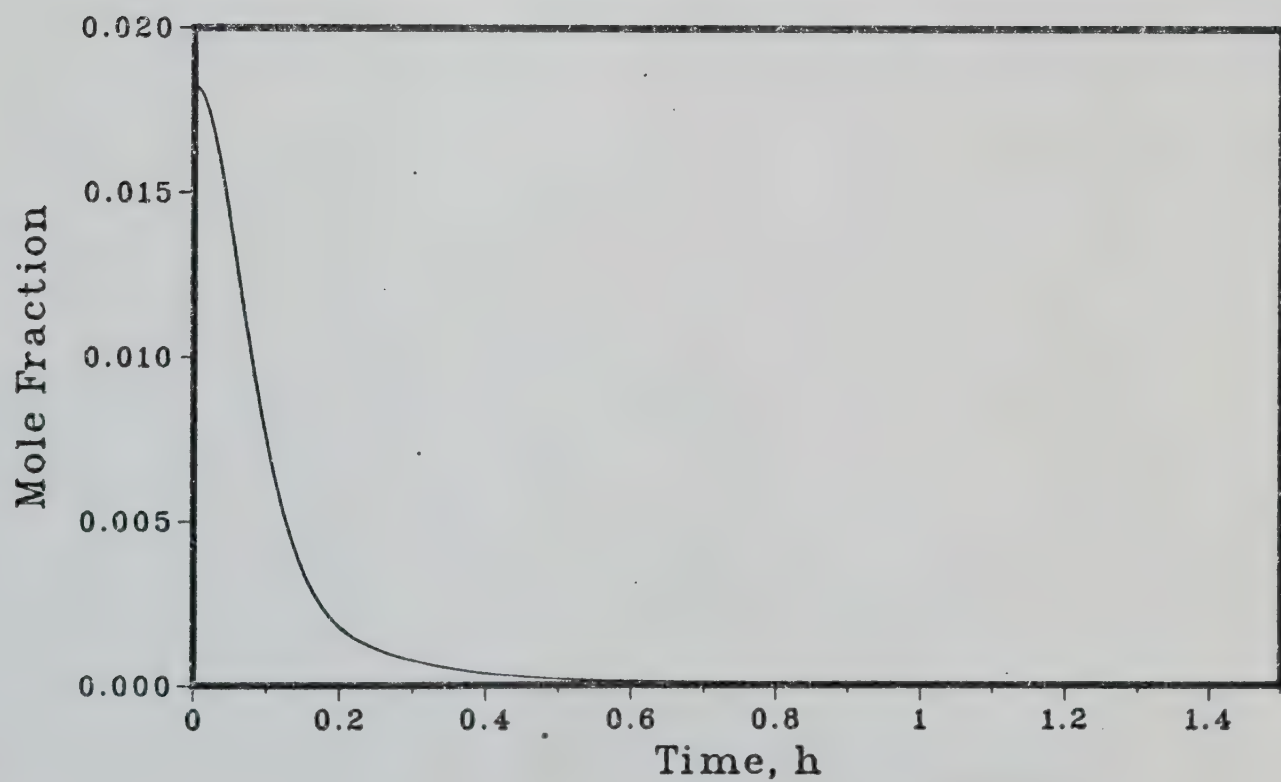


Fig. 6.16: Response of Acetone in Bottoms Product to Decrease in Temperature Set Point

Table 6.5
Response Characteristics Using Different Controller
Parameters

Test	overshoot, %	rise time, h	settling time, h
GL.TP.CL07	75.2	0.13	1.00
GL.TP.CL08	34.9	0.10	0.23

the reflux ratio is at 2.5, which means about 71% of the vapor entering the condenser is returned to the column. On the other hand, during the simulation, the reflux rate is held constant. Therefore the heat input to the reboiler must be above a certain level in order to send enough vapor to the top of the column to maintain the desired reflux, otherwise the distillate receiver will eventually run dry. From the results of some trial tests, the controller parameters in both tests GL.TP.CL07 and GL.TP.CL08 were found to cause too much decrease in the heat input rate and thus terminate the execution of the simulation prematurely. To solve this problem the proportional gain and the reset rate are reduced in the master loop for a test (GL.TP.CL11) in which the set point is decreased from 346.81K to 345.81K. The new parameters become

$$Kp_6 = 0.70$$

$$\tau_6 = 8.00 \text{ min.}$$

$$Kp_4 = 0.60$$

$$\tau_4 = 0.25 \text{ min.}$$

gave rise to the temperature response plotted in Figure 6.17. The manipulated variable response is shown in Figure 6.18. It should be noted that unlike the case for temperature set point increase, the temperature set point in this test is decreased by only 1 Kelvin. The reason is that too large a decrease will also cause the heat input to decrease below the aforementioned level even with smaller proportional gains and reset rates, and the distillate

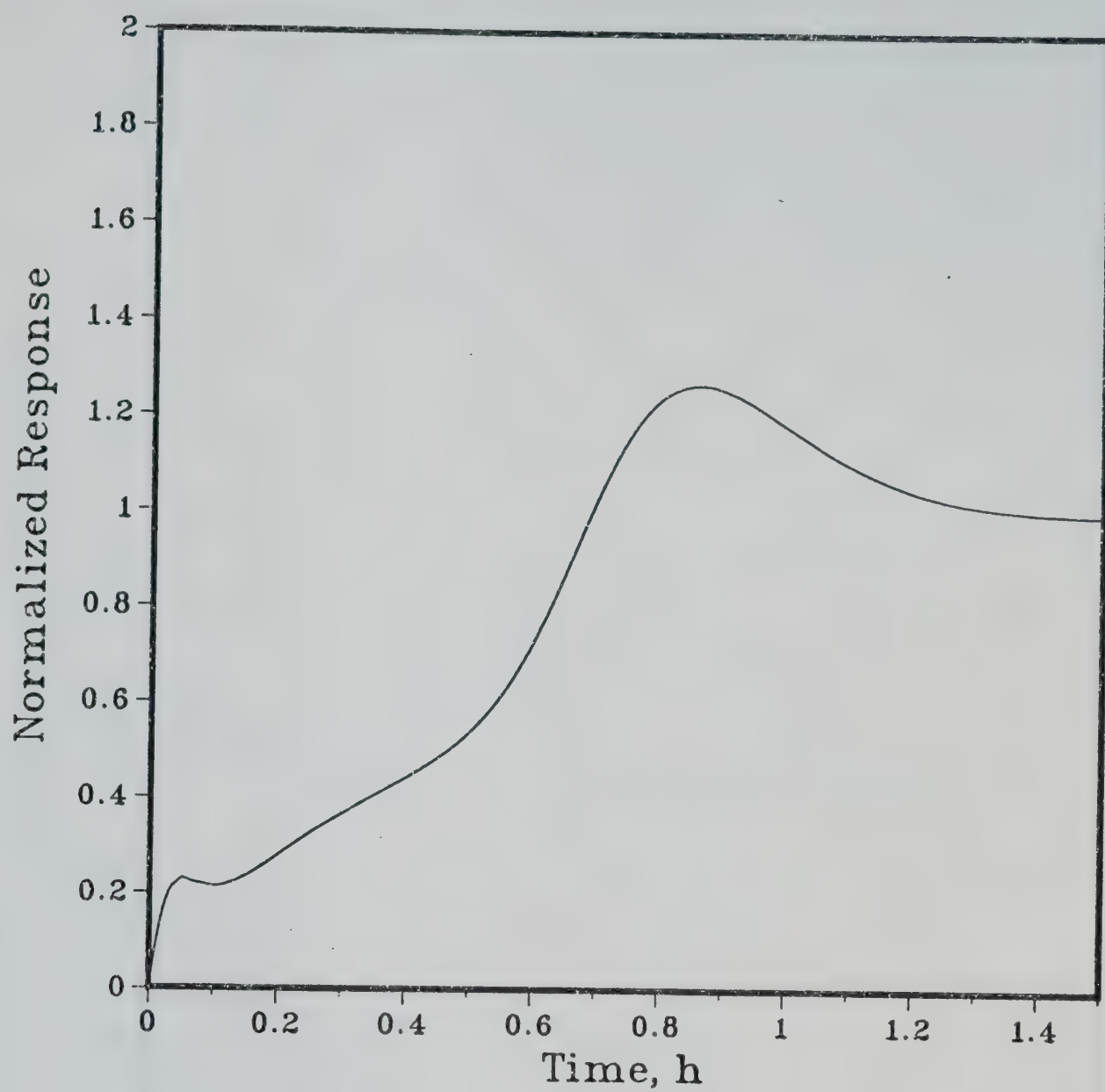


Fig. 6.17: Temperature Response of Stage 35 to Decrease in Temperature Set Point

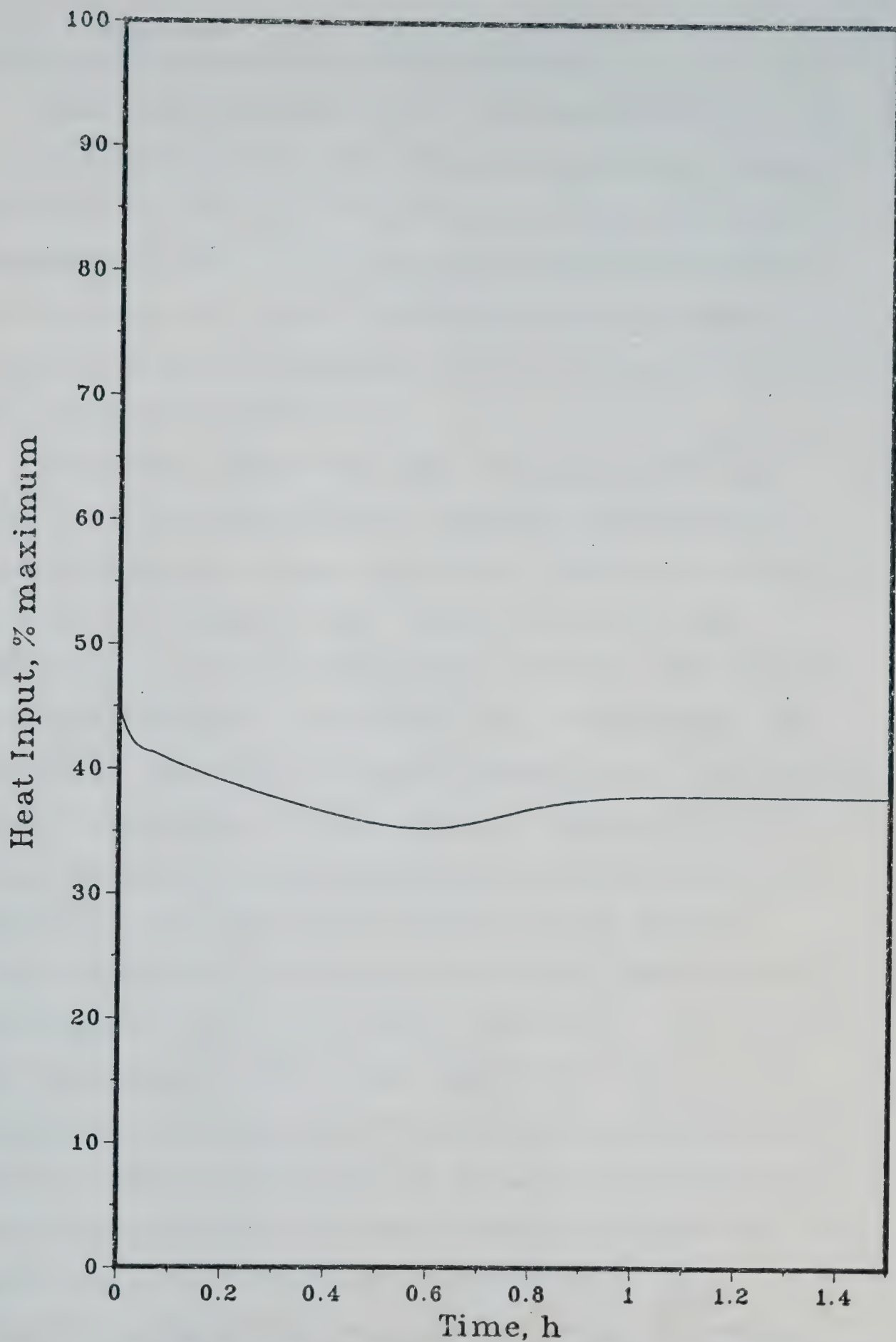


Fig. 6.18: Heat Input Response to Decrease in Temperature Set Point

receiver will be eventually dry of liquid.

Because of the necessity for the use of smaller controller gains, the closed loop performance for set point decreases will not be as satisfactory as for a set point increase. In fact, it is difficult to decrease the set point by more than one or two degrees and still have satisfactory performance unless the controller gains are even smaller than those used.

In summary, some of the open loop and closed loop dynamics of the extractive distillation column has been explored using the dynamic simulator, although the scope of the study is limited to heat input disturbances and temperature set point changes only. However, the value of the dynamic simulator, especially for process design and control, is clearly seen from the simulations. For example, one may investigate into the dynamic response of the column using the dynamic simulator before actually decreasing the temperature set point of the column. Based on the simulation results one may predict whether the decrease will be detrimental to the continuous operation of the column, such as causing the distillate receiver to run dry. Moreover, the process control engineers can apply different control schemes to overcome the difficulties encountered in temperature set point decrease. This can be done using the dynamic simulator without actually modifying the distillation column whenever a new scheme is implemented.

7. Simulation of an Industrial Distillation Unit

This chapter is concerned with the steady state and dynamic simulation of an existing industrial distillation unit. The unit at the Edmonton plant of Celanese Canada, Inc. consists of two columns, linked together such that the two columns can be represented mathematically by a model of a single column consisting of 75 trays. The unit is used to separate a mixture containing 10 nonideal chemical species. Information concerning the normal operating conditions as well as the compositions of the feed and the products have been provided by Celanese Canada Inc..

7.1 Description of the Distillation Unit

The distillation unit consists of two separate columns, denoted by column "A" and column "B". Column "A" has 40 trays and a reboiler for a total of 41 stages. The reboiler is supplied with steam as the heating medium. The feed stream enters the column at a location near the top of the column. The vapor leaving the top tray of column "A" is directed to the bottom of column "B", which consists of 35 trays and a water cooled, total condenser. The liquid leaving the bottom of column "B" is pumped back to the top tray of column "A". Therefore, for simulation purpose, the distillation unit can be modelled as a single column consisting of 75 trays plus a reboiler and a total condenser, although the characteristic dimensions of the trays are not necessarily the same in both columns.

7.2 Simulation of the Initial Steady State

From the information on some of the variables of the column at normal operating conditions, an initial steady state is computed. In the computation, a reflux ratio of 4.40, an overall tray efficiency of 0.47 and a heat input rate of 947.5 kW are used so that the calculated product compositions and flow rates are as close to the given information as possible.

The properties of the feed stream are given in Table 7.1, and the calculated product compositions and flow rates are compared values specified by Celanese Canada in Table 7.2. In Table 7.3, the steady state value of some of the variables are listed.

The simulation results shown in Table 7.2 indicate that a large discrepancy exists in both the distillate temperature and the bottom product pressure. The discrepancy in the distillate temperature is due to the fact that the calculated temperature is the equilibrium temperature of the distillate, whereas the measured temperature is obtained from the subcooled liquid inside the distillate receiver. The calculated temperatures at the other trays match more closely with the actual temperature, as exemplified by the fact that the calculated temperature of the top tray of column "B" is 360.48 K, whereas the measured temperature is 365 K. However, the calculated profile is still consistently below the measured temperatures by several degrees in Kelvin. The probable

Table 7.1
Distillation Unit Feed Specification

Component	Composition
1	0.2838
2	0.0563
3	0.0387
4	0.0234
5	0.0784
6	0.0345
7	0.0893
8	0.2894
9	0.0819
10	0.0243

Flow rate = 27.2 mol/s

Temperature = 360.0 K

Table 7.2

Comparison of the Calculated Product Properties to the Measured Properties

Property	Distillate		Bottoms	
	Calculated	Measured	Calculated	Measured
x_1	0.0504	0.0756	0.3480	0.3429
x_2	0.1414	0.1700	0.0326	0.0241
x_3	0.1780	0.1751	0.0000	0.0000
x_4	0.1075	0.1058	0.0001	0.0000
x_5	0.0162	0.0000	0.0960	0.1006
x_6	0.1025	0.0938	0.0154	0.0177
x_7	0.3661	0.3798	0.0120	0.0069
x_8	0.0067	0.0000	0.3686	0.3713
x_9	0.0311	0.0000	0.0962	0.1052
x_{10}	0.0000	0.0000	0.0310	0.0313
Temperature, K	357.59	315	387.53	396
Pressure, kPa	338.0	338	389.49	414
Flow rate, kg/s	0.3416	0.333	1.104	1.111

Table 7.3

Selected Steady State Variables at the Initial Steady State

Stage	T_j, K	P_j, kPa
1	357.59	338.00
5	365.42	340.51
10	369.77	344.59
15	373.55	348.48
20	376.12	352.22
25	377.52	355.86
30	378.35	359.44
35	379.01	362.98
40	379.49	366.13
45	380.03	369.10
50	381.47	372.35
55	382.50	375.59
60	383.43	378.80
65	384.36	381.99
70	385.43	385.14
75	386.67	388.25
77	387.53	389.49

Stage	M_j, mol	$L_j, mol/s$	$V_j, mol/s$
1	12523	26.4	0.00
5	509	26.1	32.3
10	508	25.3	31.5
15	510	24.5	30.7
20	513	24.1	30.2
25	517	24.0	30.0
30	521	24.0	30.0
35	526	24.0	30.0
40	595	24.0	30.0
45	682	54.3	32.6
50	682	54.4	32.7
55	682	54.4	32.7
60	683	54.3	32.6
65	684	54.3	32.6
70	684	54.1	32.5
75	686	54.0	32.3
77	14800	21.7	32.3

reason is the inability of the equilibrium model to represent the mixture with high accuracy. In order to reduce the magnitude of the error, experimental data for the mixture are much needed so that the thermodynamic parameters, the Wilson interaction energy parameter in particular, can be adjusted.

The error in the calculated pressure of the bottoms product, and possibly in most of the trays, is because of the assumption that the pressure loss across each tray is caused only by the dry pressure drop and the hydraulic head loss (cf Chapter 6). Other factors that contribute to additional pressure loss, which are ignored in modelling column behavior, such as the pressure loss for overcoming surface tension as the vapor rises from a perforation, may have considerable effect on the tray pressure profile of the columns. If all the significant factors contributing to pressure drop were incorporated into the model, such that the gradient of the pressure profile becomes larger, the calculated temperature of the bottom product would likely be higher. It should also be noted that the calculated pressure of the distillate has no error since the pressure is set equal to the measured value to serve as the reference for the calculation of the pressure on the trays below the condenser.

7.3 Simulation for the Dynamic Behavior

Dynamic simulation was performed for various types of disturbances to illustrate the transient behavior of the column. The types of disturbance are step changes in the feed flow rate, the heat input rate and the reflux rate.

In the simulation, the column is assumed to be at the steady state as described in the previous section. The simulation was performed with the assumptions that the overall tray efficiency is at a constant value of 0.47, and that the holdups at the condenser stage and the reboiler stage are constant at 12.5 kmol and 14.8 kmol, respectively. The heat input rate to the reboiler was set to a constant value of 947.5 kW, except for the case of step changes in the heat input rate. Heat loss to the environment is assumed negligible. In the following sections, the dynamic response of the distillation unit to each type of disturbance is discussed.

7.3.1 Simulation for Step Changes in Feed Flow Rate

In this simulation, the feed flow rate is perturbed from the initial rate of 27.7 mol/s at time 0⁻ with different magnitudes as shown in Table 7.4. The dynamic response of the tray temperatures that results from these changes is characterized by nonminimum phase behavior and a large range of response times. As can be seen in Figures 7.1 to 7.4, the nonminimum phase behavior of the temperatures is especially noticeable for increases in feed

Table 7.4
Feed Flow Rate After Time 0⁻

Test	% Change	New Flow Rate mol/s
CL.FD.OL17	+15	31.9
CL.FD.OL18	-15	23.5
CL.FD.OL19	+30	36.0
CL.FD.OL20	-30	19.4

flow, and the response times are much longer than those for decreases in the feed flow. It can be observed that the nonminimum phase behavior progresses downwards from the condenser stage and reaches a maximum in the vicinity of stage 45. Further down from stage 45, the nonminimum phase behavior appears to damp out gradually. Large shifts in the steady state profile of temperature and compositions are also observed from the simulation results, although the shifts in the products are considerably less than those in the intermediate stages of the distillation unit. From the steady state profiles in Figures 7.5 to 7.6, it can be seen that the shifts are quite nonlinear, and the range of composition gradient is very large. The inverse response maps in Tables 7.5 to 7.6 for +30% and -30% change, respectively, indicate that the inverse response behavior exists frequently in the compositions on the intermediate stages of the distillation unit, and that neither temperature nor product compositions show any inverse response behavior except the composition of C_7 and C_{10} in

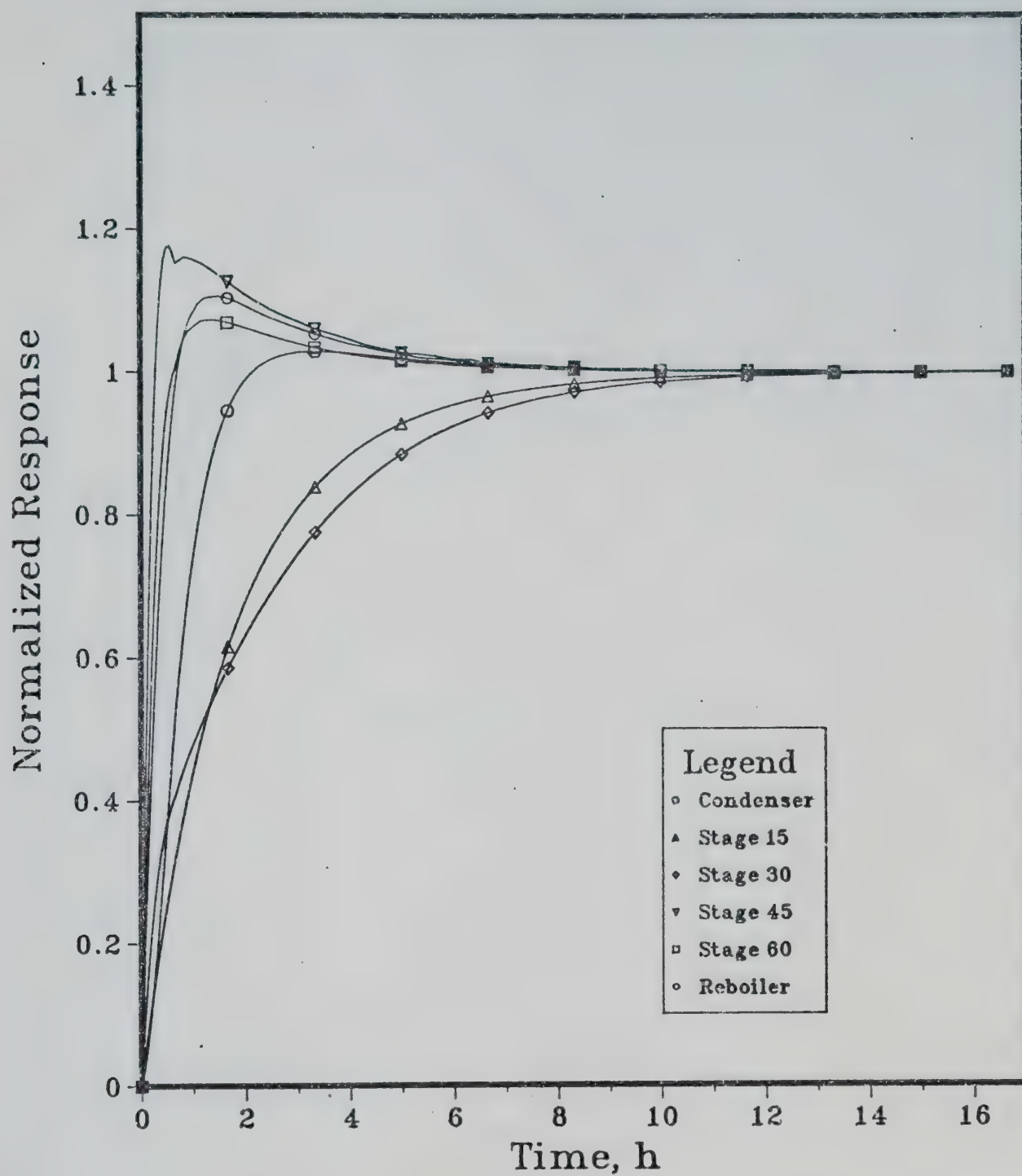


Fig. 7.1 Normalized Response of Stage Temperatures to a +15% Step Change in Feed Flow Rate

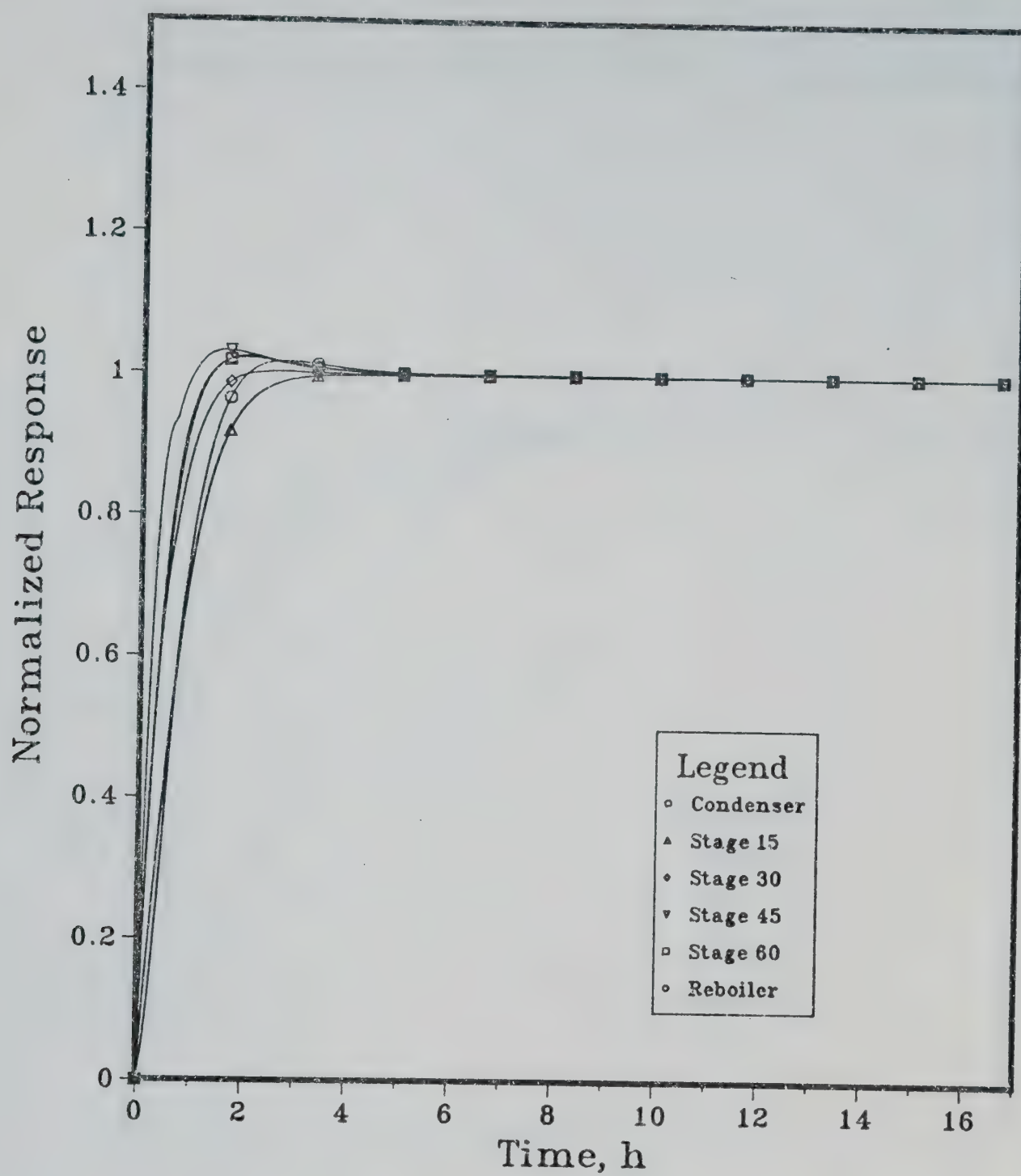


Fig. 7.2 Normalized Response of Stage Temperatures to a -15% Step Change in Feed Flow Rate

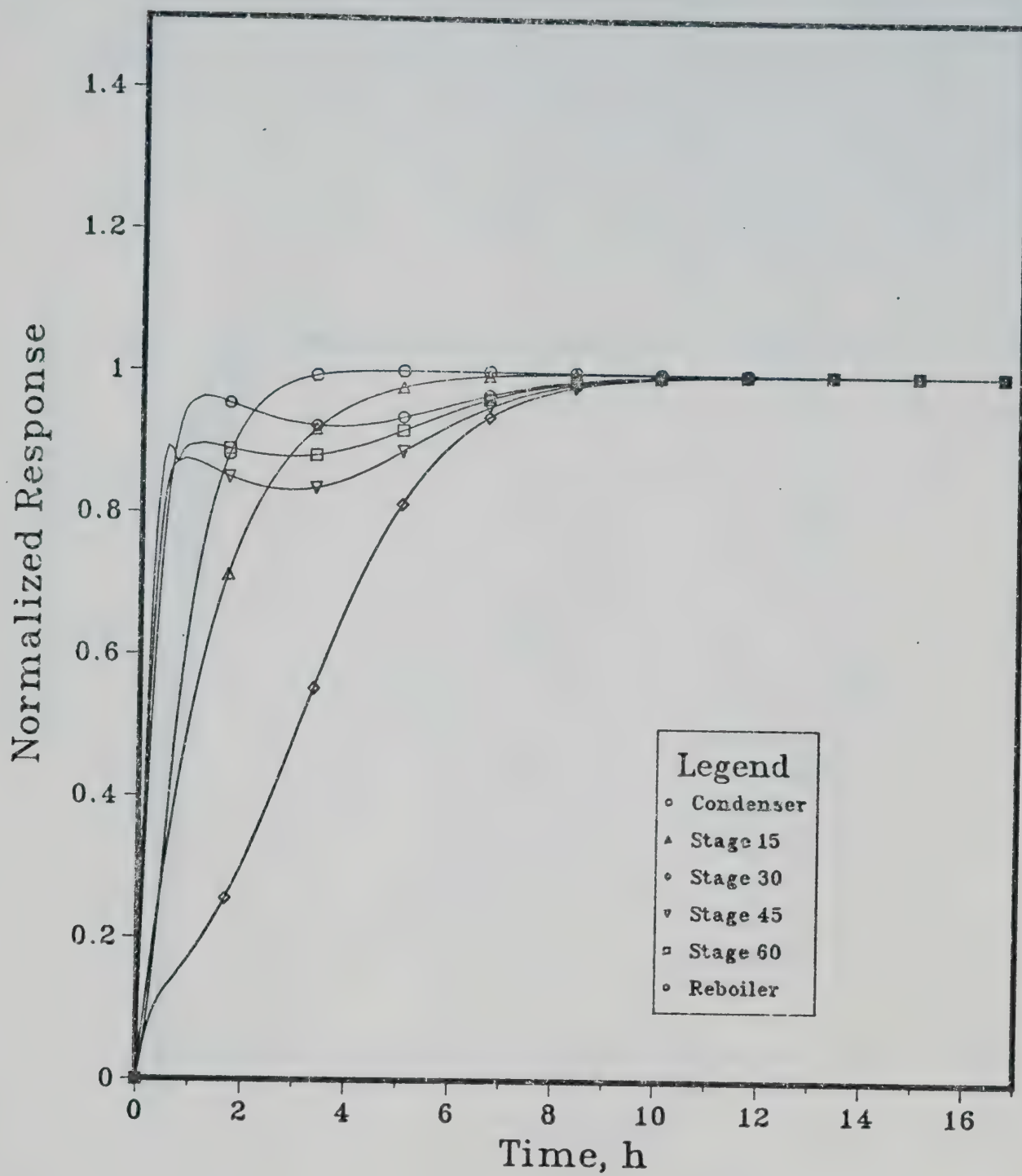


Fig. 7.3 Normalized Response of Stage Temperatures to a +30% Step Change in Feed Flow Rate

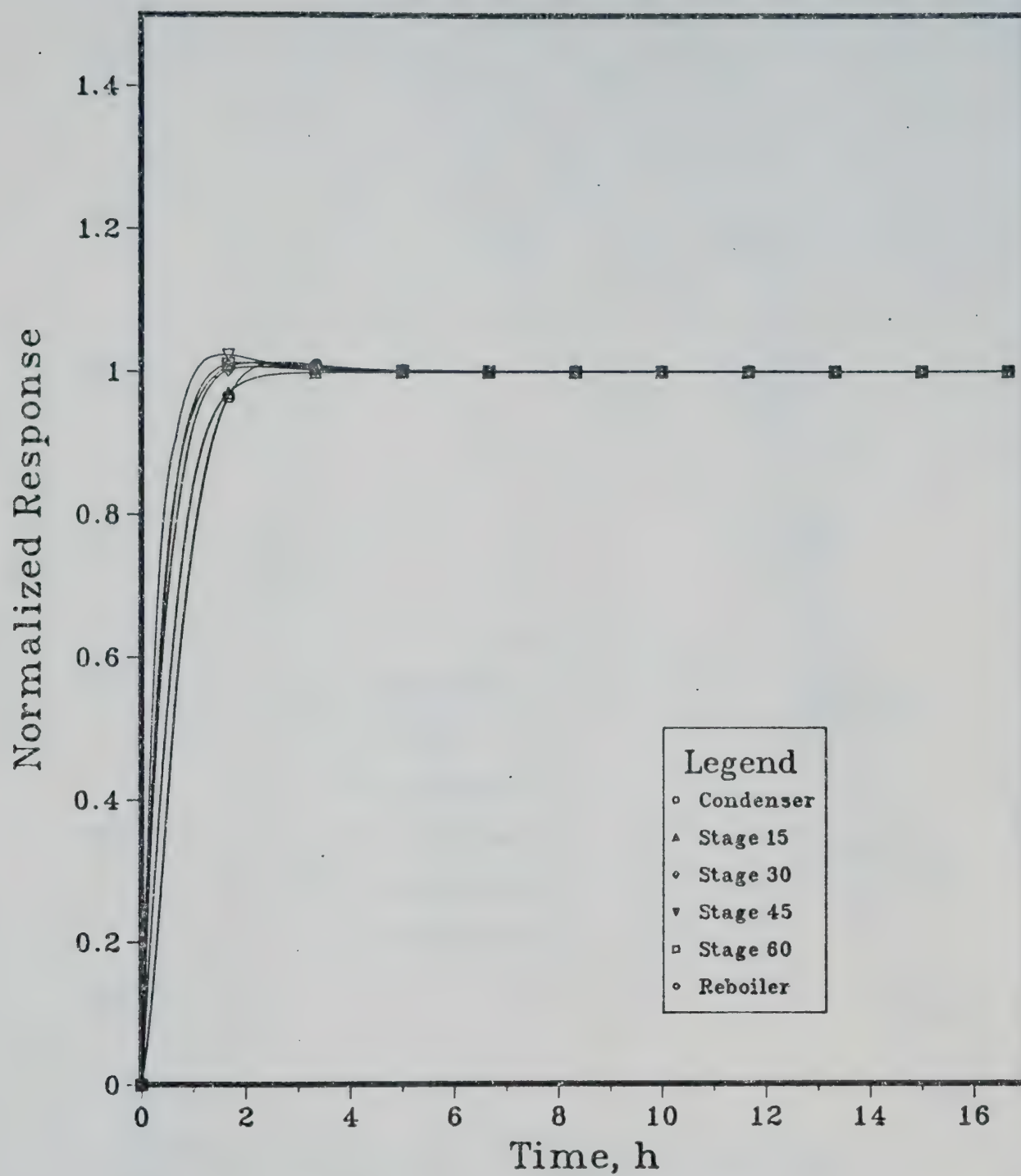


Fig. 7.4 Normalized Response of Stage Temperatures to a -30% Step Change in Feed Flow Rate

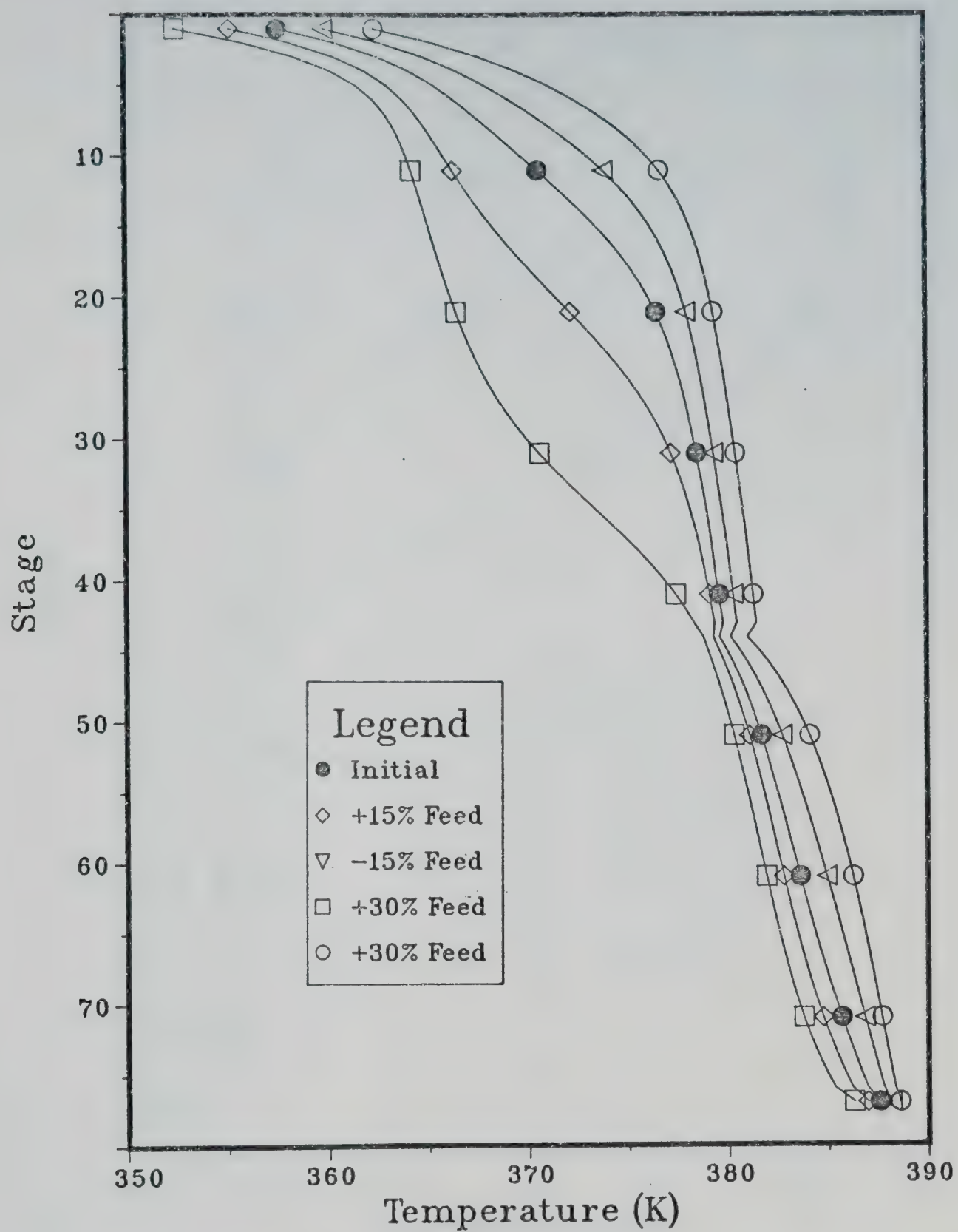


Fig. 7.5 Steady State Temperature Profiles for Changes in Feed Flow Rate

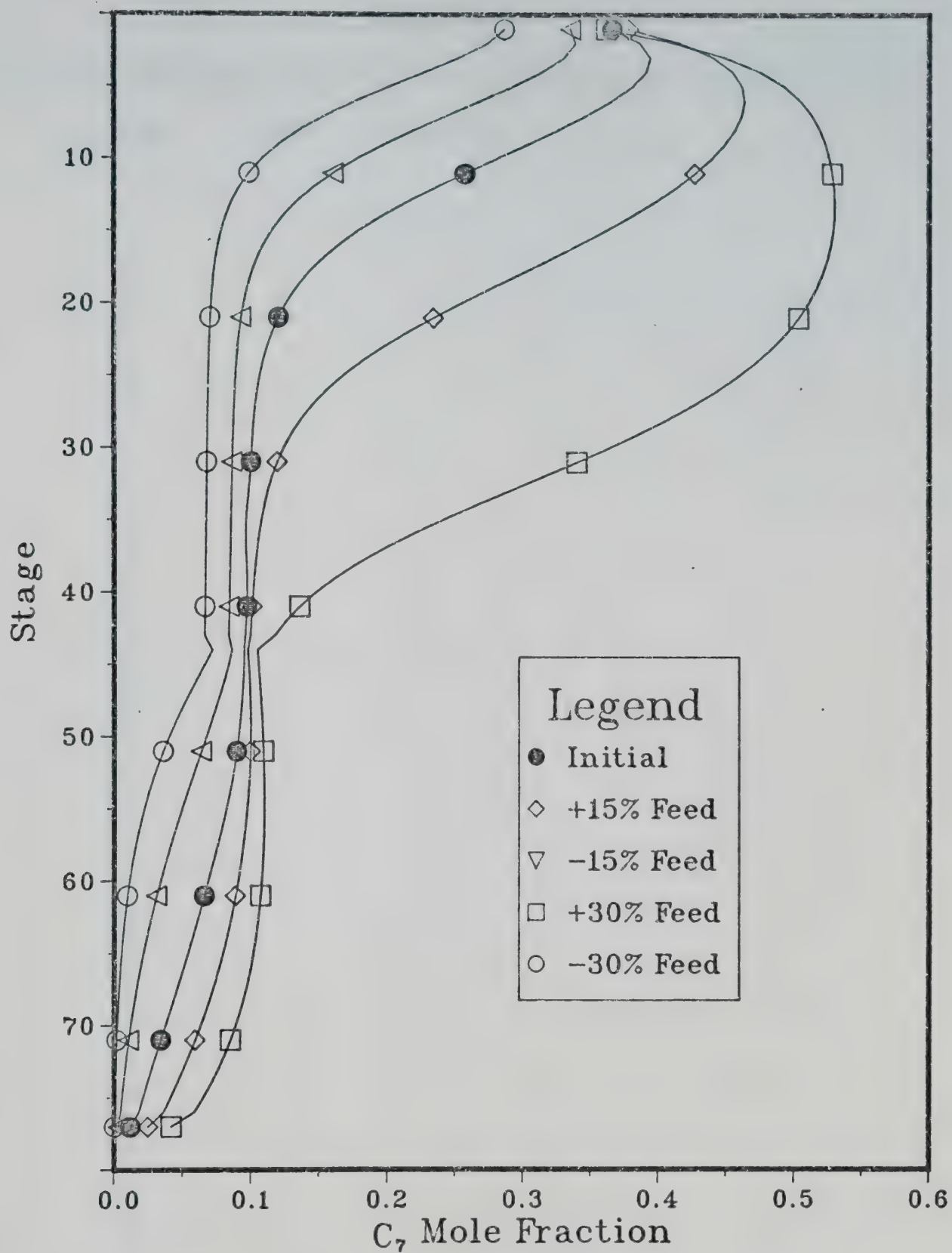


Fig. 7.6 Steady State C_7 Composition Profiles for Changes in Feed Flow Rate

Table 7.5

Inverse Response Map for a +15% Change in Feed Flow Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	.	.	.	.	.	*	.	.	.
3	.	.	*	.	.	.	*	.	.	.	.
5	.	.	.	.	.	.	*	.	.	.	.
7	.	.	.	.	.	.	.	.	.	.	.
9	.	.	.	.	.	.	.	.	.	.	.
11	.	.	.	.	.	.	.	.	.	.	.
13	.	.	.	.	.	.	.	.	.	.	.
15	.	.	.	.	.	.	.	.	.	.	.
17	.	.	.	.	.	.	.	.	.	.	.
19	.	.	.	.	.	.	.	.	.	.	.
21	.	.	.	.	.	.	.	.	.	*	.
23	.	.	.	.	.	.	.	.	.	*	.
25	.	.	.	.	.	.	.	.	.	.	.
27	.	.	*	.	.	*	.	.	.	.	.
29	.	.	*	.	.	*	.	.	.	.	.
31	.	.	*	.	.	*	*	.	.	.	.
33	.	.	*	.	.	*	*	.	.	.	.
35	.	.	*	.	.	*	*	.	.	.	.
37	.	.	*	.	.	*	*	.	*	.	.
39	.	.	*	.	.	*	*	.	*	.	.
41	.	.	*	.	.	*	*	.	.	.	.
43	.	.	.	.	.	.	.	.	.	*	.
45	.	.	.	.	.	.	.	.	.	*	.
47	.	.	.	.	.	.	.	.	.	*	.
49	.	.	.	.	.	.	.	.	.	*	.
51	.	.	.	.	.	.	.	.	.	.	.
53	.	.	.	.	.	.	.	.	.	.	.
55	.	.	.	.	.	.	.	.	.	.	.
57	.	.	.	.	.	.	.	.	.	.	.
59	.	.	.	.	.	.	*	.	.	.	.
61	.	.	.	.	.	.	.	.	.	.	.
63	.	.	.	.	.	.	.	.	.	.	.
65	.	.	.	.	.	.	.	.	.	.	.
67	.	.	.	.	.	.	.	.	.	.	.
69	.	.	.	.	.	.	.	.	.	.	.
71	.	.	.	.	.	.	.	.	.	.	.
73	.	.	.	.	.	.	.	.	.	.	.
75	.	.	.	.	.	.	.	.	.	.	.
77	.	.	.	.	.	*	.	.	.	*	.

* - inverse response
 . - normal response

Table 7.6

Inverse Response Map for a -15% Change in Feed Flow Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	.	.	.	.	.	*	.	.	.
3	.	.	*	.	.	.	.	.	.	.	.
5	.	.	.	.	.	.	*	.	.	.	*
7	.	.	.	.	.	.	.	.	.	.	*
9	.	.	.	.	.	.	.	.	.	.	.
11	.	.	.	.	.	.	.	.	.	.	.
13	.	.	.	.	.	.	.	.	.	.	.
15	.	.	.	.	.	.	.	.	.	*	.
17	.	.	.	.	.	.	.	.	.	*	.
19	.	.	.	.	.	.	.	.	.	*	.
21	.	.	.	.	.	.	.	.	.	.	.
23	.	.	.	.	.	.	.	.	.	.	.
25	.	.	.	.	.	.	.	.	.	.	.
27	.	.	.	.	.	.	*	.	.	.	.
29	.	.	.	.	.	.	*	.	.	.	.
31	.	.	*	.	.	.	*	.	.	.	.
33	.	.	*	.	.	.	*	.	.	.	.
35	.	*	.	.	.	.	.	.	.	*	.
37	.	.	*	.	.	.	.	.	.	*	.
39	.	*	.	.	.	.	.	.	.	*	.
41	.	.	.	.	.	*	*	.	.	*	.
43	.	.	.	.	.	.	.	.	.	*	.
45	.	.	.	.	.	.	.	.	.	.	*
47	.	.	.	.	.	.	.	.	.	.	*
49	.	.	*	.	.	.	*	.	.	.	*
51	.	.	*	.	.	.	*	.	.	.	.
53	.	.	.	.	.	.	*	.	.	.	.
55	.	.	.	.	.	.	.	.	.	.	.
57	.	.	.	.	.	.	.	.	.	.	.
59	.	.	.	.	.	.	.	.	.	.	.
61	.	.	.	.	.	.	.	.	.	.	.
63	.	.	.	.	.	.	.	.	.	.	.
65	.	.	.	.	.	.	.	.	.	.	.
67	.	.	.	.	.	.	.	.	.	.	.
69	.	.	.	.	.	.	.	.	.	.	.
71	.	.	.	.	.	.	.	.	.	.	.
73	.	.	.	.	.	.	.	.	.	.	.
75	.	.	.	.	.	.	.	.	.	*	.
77	.	.	.	.	.	.	.	.	.	.	.

* - inverse response
. - normal response

the top product. It should be noted that the stages where most compositions show inverse response behavior are the locations where the nonminimum phase characteristic of the temperature is most prominent.

7.3.2 Simulation for Step Changes in Heat Input Rate

Simulation of column behavior for heat input changes involves step changes in the heat input rate from the initial value of 947.5 kW. The new heat input rates are tabulated in Table 7.7 for the different tests.

Table 7.7
Heat Input Rate After Time 0⁻

Test	% Change	New Heat Input Rate, kW
CL.QR.OL15	+5	994.9
CL.QR.OL16	-5	900.1
CL.QR.OL17	+10	1042.3
CL.QR.OL18	-10	852.8

The dynamic response of some of the stage temperatures are plotted in Figures 7.7 to 7.10 for the four tests listed in Table 7.7. As can be seen from these plots, the temperature response for decreases in heat input rate exhibits significant nonminimum phase behavior on most of the stages below stage 30, and the response times are generally longer than those corresponding to increases in the heat input

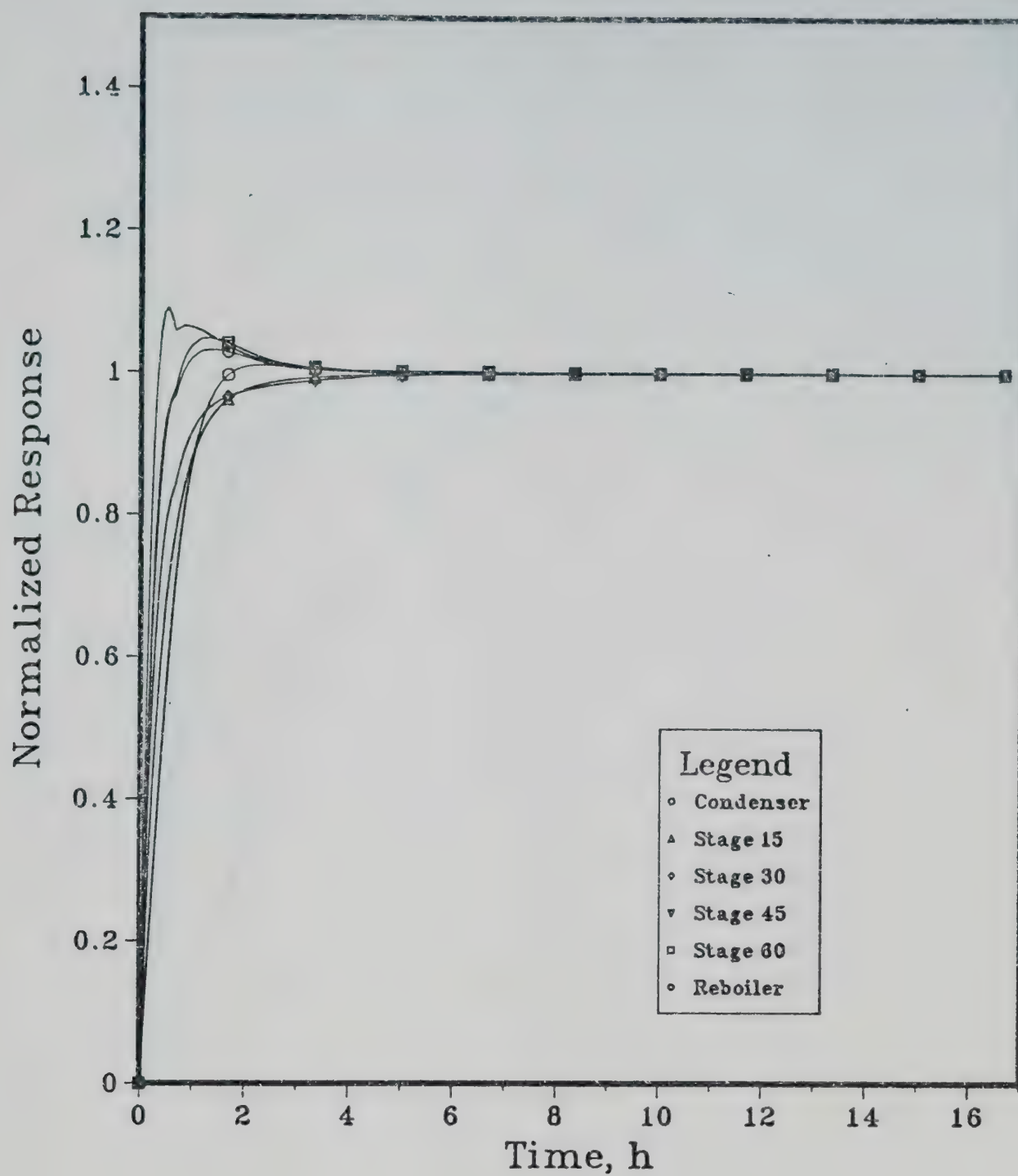


Fig. 7.7 Normalized Response of Stage Temperatures to a +5% Step Change in Heat Input Rate

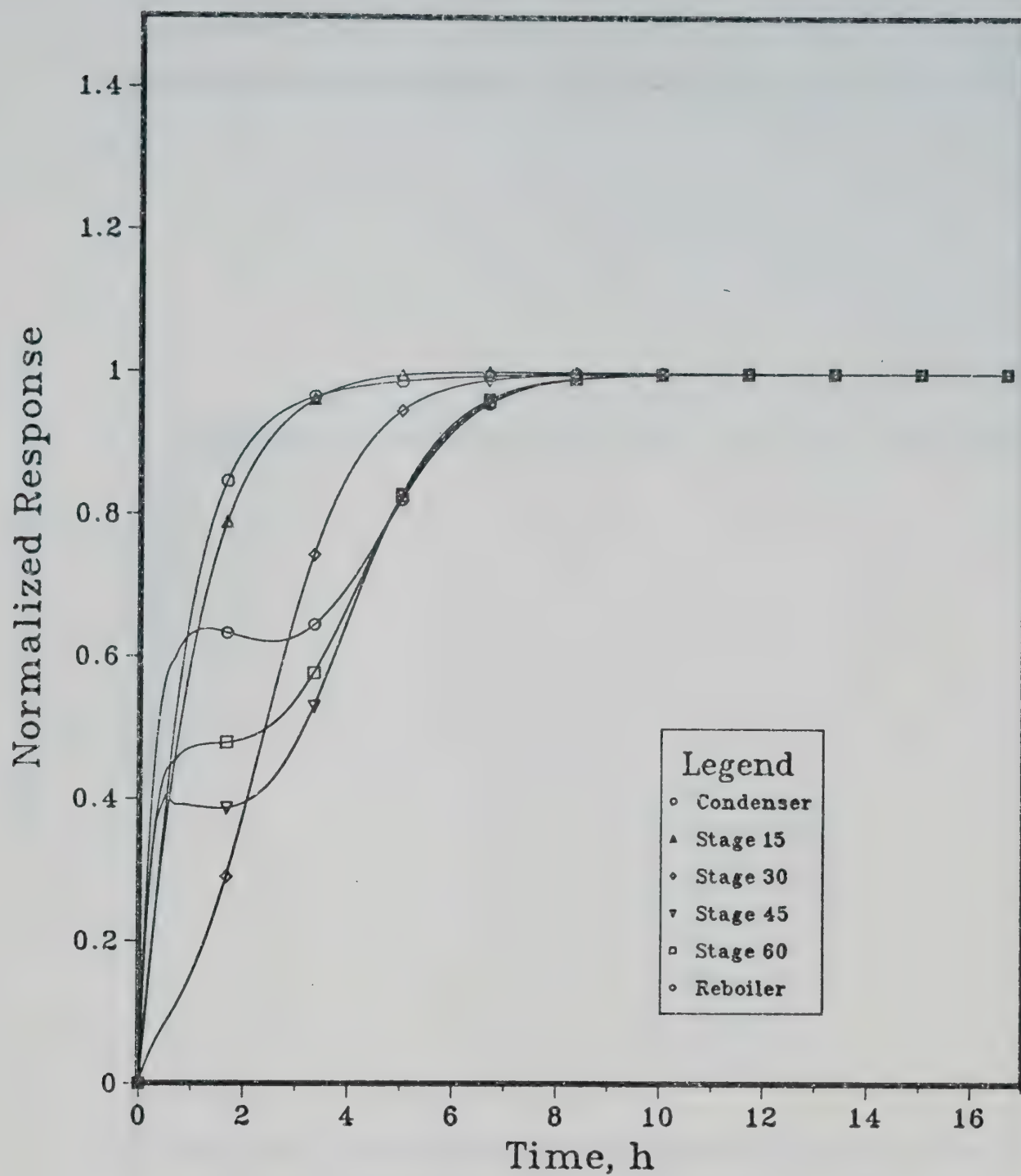


Fig. 7.8 Normalized Response of Stage Temperatures to a -5% Step Change in Heat Input Rate

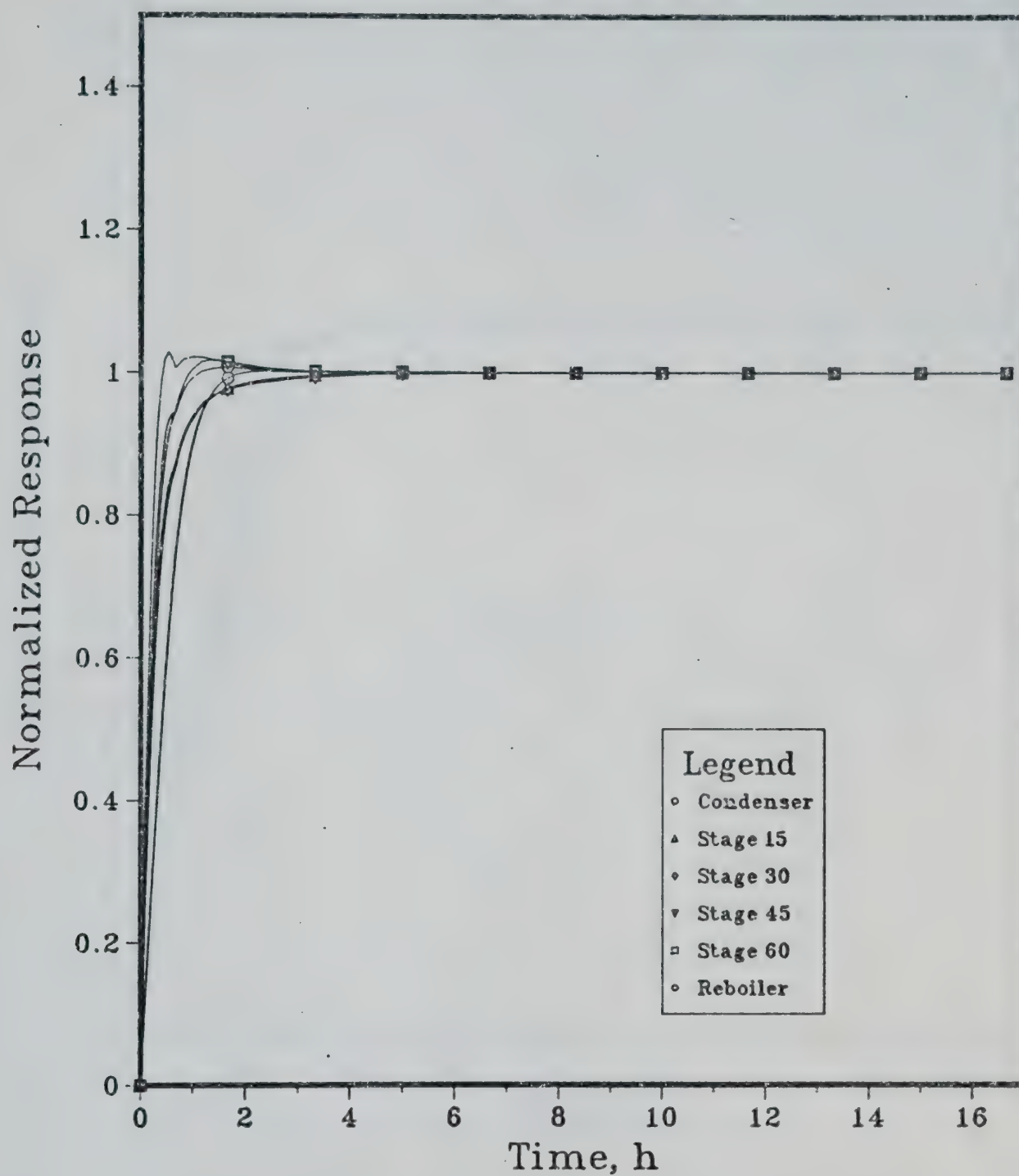


Fig. 7.9 Normalized Response of Stage Temperatures to a +10% Step Change in Heat Input Rate

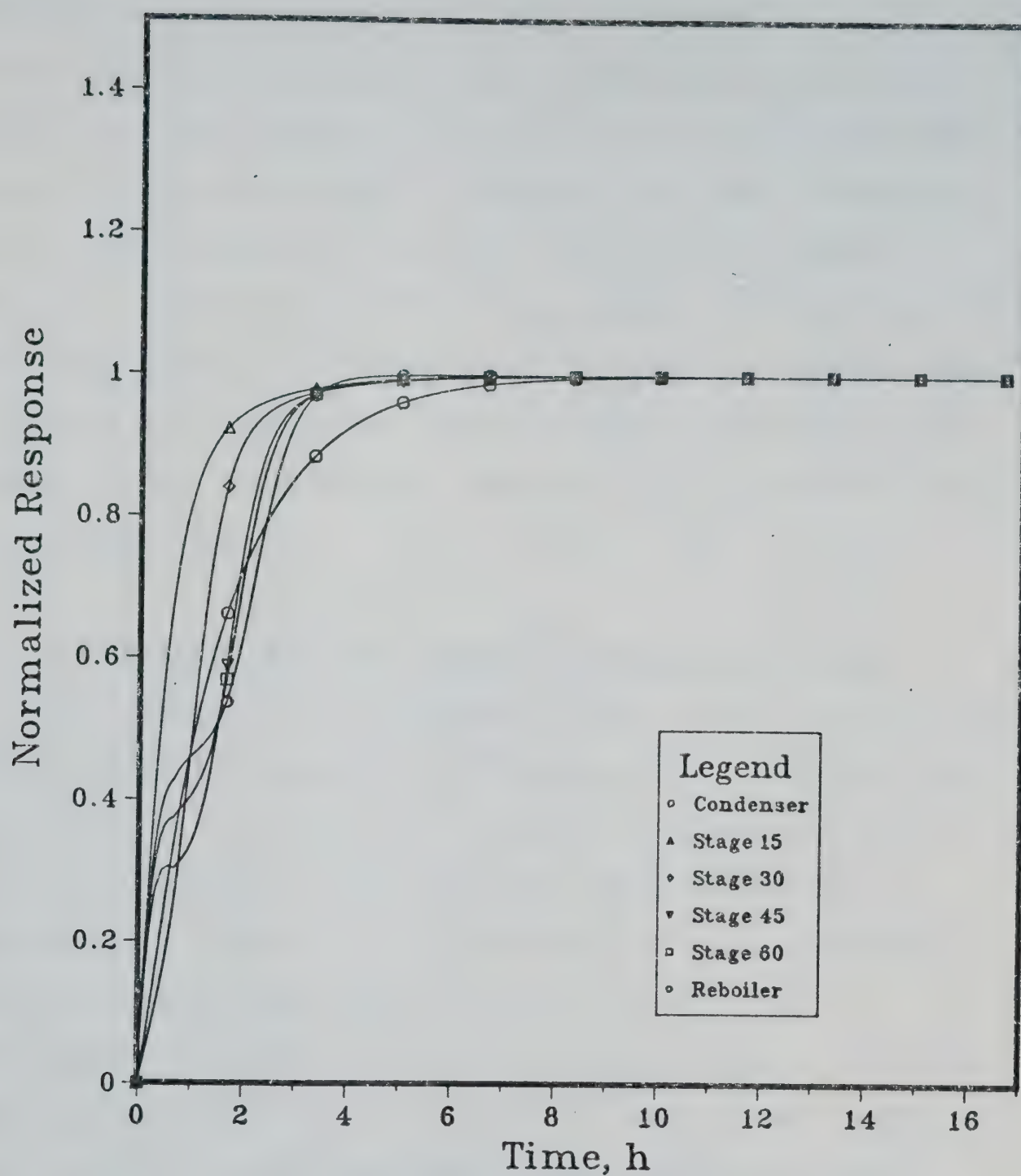


Fig. 7.10 Normalized Response of Stage Temperatures to a -10% Step Change in Heat Input Rate

rate. The shifts in the steady state profiles of temperatures and compositions, as illustrated in Figures 7.11 to 7.12, are large for decreases in the heat input rate, and the amount of shift is very nonlinear with respect to the magnitude of change of the input, especially in the upper stages of the distillation unit. Inverse response behavior is exhibited by a number of components on various stages, as illustrated by the inverse response maps in Tables 7.8 and 7.9 for tests CL.QR.OL17 and CL.QR.OL18 respectively, although such behavior is not observed in any stage temperature.

7.3.3 Simulation for Step Changes in Reflux Flow Rate

The simulation for changes in the reflux flow rate are conducted by introducing step changes of various magnitudes in the molar flow rate of the reflux recycled to column "B" of the distillation unit. The new reflux rates, as tabulated in Table 7.10, introduced at time 0⁻, replace the initial steady state value of 26.43 mol/s.

The dynamic response of the stage temperatures to the reflux flow disturbance is quite similar to that to heat input disturbances in that nonminimum phase behavior is very apparent in most trays below stage 30. As seen from Figures 7.13 to 7.16, the nonminimum phase behavior is especially pronounced for increases in the reflux flow rate. This result is apparently consistent with the observation that the behavior is more significant for decreases in heat

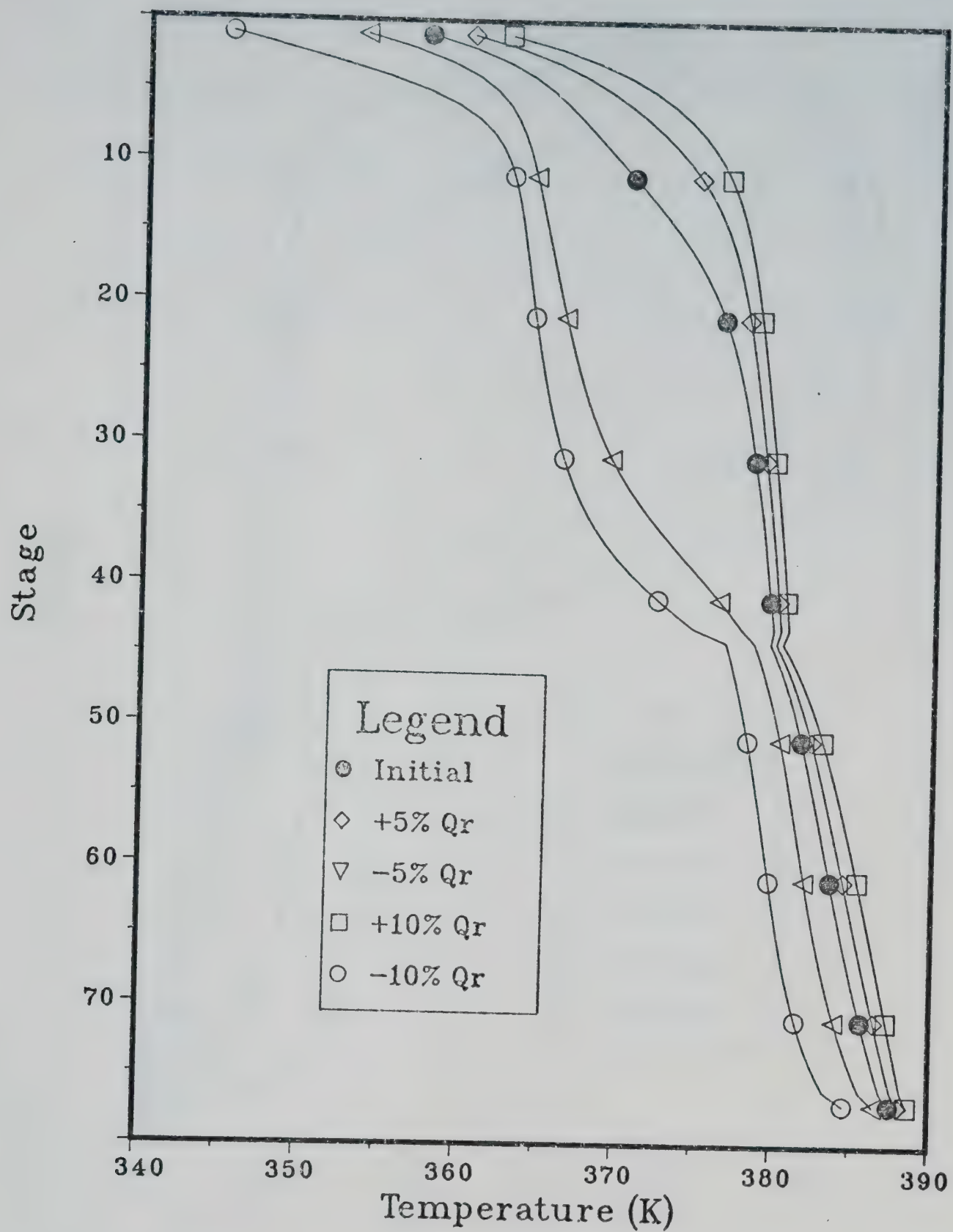


Fig. 7.11 Steady State Temperature Profiles for Changes in Heat Input Rate

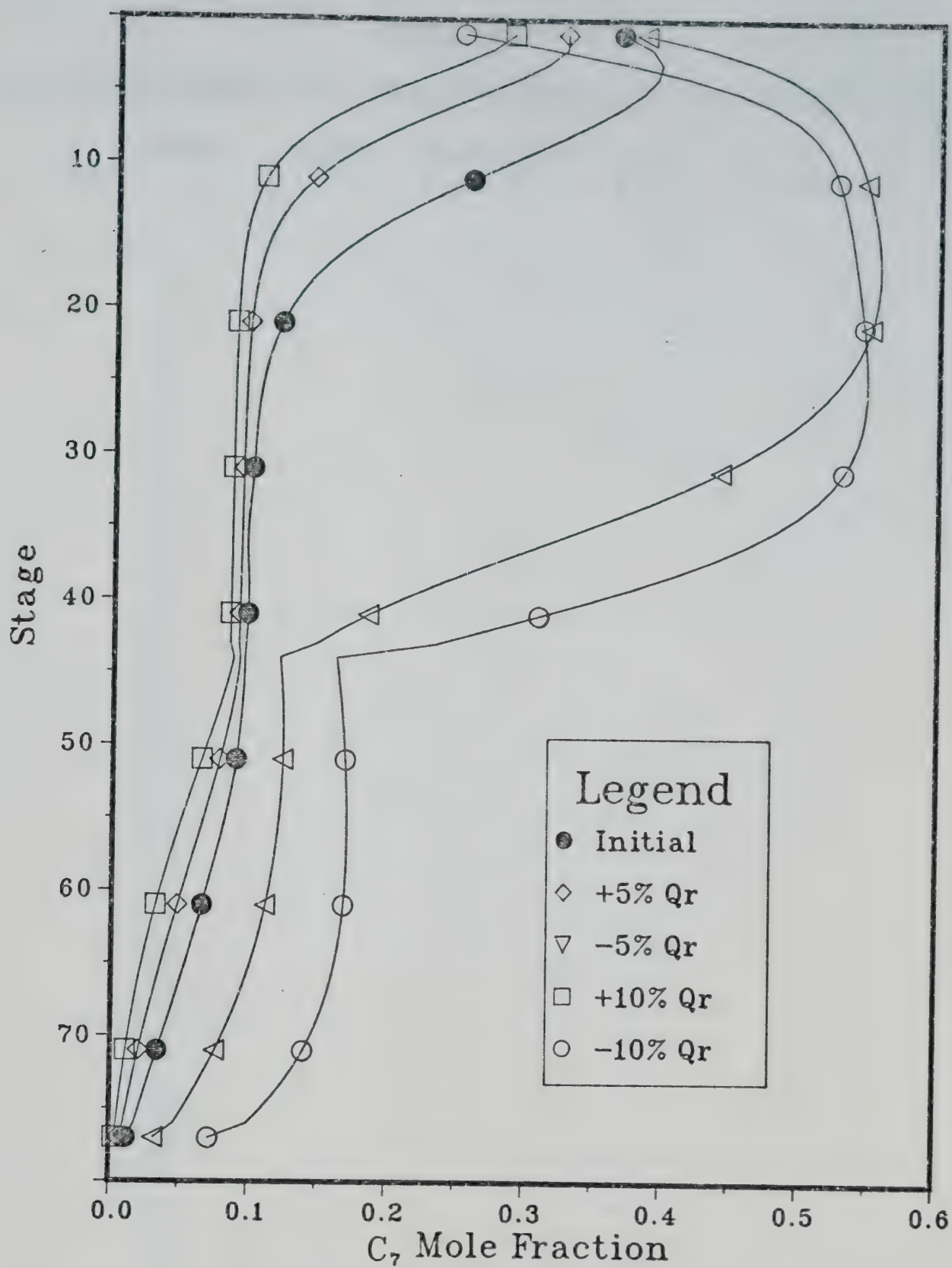


Fig. 7.12 Steady State C_7 Composition Profiles for Changes in Heat Input Rate

Table 7.8

Inverse Response Map for a +5% Change in Heat Input Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	*	.	.	.	*	.	.	.	.
3	.	.	.	.	.	.	.	.	.	.	.
5	.	.	.	.	.	.	.	.	.	.	.
7	.	.	.	.	.	.	.	.	.	.	.
9	.	.	.	.	.	.	.	.	.	.	.
11	.	.	.	.	.	.	.	.	.	*	.
13	.	.	.	.	.	.	.	.	.	*	.
15	.	.	.	.	.	.	.	.	.	*	.
17	.	.	.	.	.	.	.	.	.	.	.
19	.	.	.	.	.	*	.	.	.	.	.
21	.	.	.	.	.	.	.	.	.	.	.
23	.	.	.	.	*	.	.	.	.	.	.
25	.	.	.	.	*	.	.	.	.	.	.
27	.	.	.	.	*	.	.	.	.	.	.
29	.	.	.	.	*	.	.	.	.	.	.
31	.	.	.	.	.	.	.	.	.	.	.
33	.	.	.	.	.	.	.	.	.	.	.
35	.	.	.	.	.	.	*	.	.	.	.
37	.	*	.	.	.	.	.	.	.	.	.
39	.	*	.	.	.	.	*	.	.	.	.
41	.	.	.	.	.	.	*	.	.	.	.
43	.	.	.	.	.	.	.	.	.	.	.
45	.	.	.	.	.	.	.	.	.	.	.
47	.	.	.	.	.	.	.	.	.	.	.
49	.	.	.	.	.	.	.	.	.	*	.
51	.	.	*	.	.	*	.	.	.	*	.
53	.	.	*	.	.	*	*	.	.	*	.
55	.	.	.	.	.	*	.	.	.	*	.
57	.	.	.	.	.	.	.	.	.	*	.
59	.	.	.	.	.	.	.	.	.	*	.
61	.	.	.	.	.	.	.	.	.	*	.
63	.	.	.	.	.	.	.	.	.	*	.
65	.	.	.	.	.	.	.	.	.	*	.
67	.	.	.	.	.	.	.	.	.	*	.
69	.	.	.	.	.	*	.	.	.	*	.
71	.	.	.	.	.	*	.	.	.	*	.
73	.	.	.	.	.	*	.	.	.	*	.
75	.	.	.	.	.	.	.	.	.	.	.
77	.	.	.	.	.	.	.	.	.	.	.

* - inverse response
. - normal response

Table 7.9

Inverse Response Map for a -5% Change in Heat Input Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	*	.	.	.	.	*	.	.	*
3	.	.	.	.	.	.	.	.	.	.	.
5	.	.	.	.	.	.	*	.	.	.	.
7	.	.	.	.	.	.	*	.	.	.	.
9	.	.	.	.	.	.	*	.	.	.	.
11	.	.	.	.	.	.	.	.	.	.	.
13	.	.	.	.	.	.	.	.	.	.	.
15	.	.	.	.	.	.	.	.	.	.	.
17	.	.	.	.	.	.	.	.	.	.	.
19	.	.	.	.	.	.	.	.	.	.	.
21	.	.	.	.	.	.	.	.	.	*	.
23	.	.	.	.	.	.	.	.	.	*	.
25	.	.	.	.	.	*	.	.	.	*	.
27	.	.	.	.	.	*	.	.	.	*	.
29	.	.	.	.	.	*	.	.	.	*	.
31	.	.	.	.	.	*	.	.	.	*	.
33	.	.	.	.	.	*	.	.	.	*	.
35	.	.	*	.	.	*	.	.	.	*	.
37	.	.	*	.	.	*	.	.	.	*	.
39	.	.	.	.	.	*	.	.	.	*	.
41	.	.	.	.	.	*	*	.	.	*	.
43	.	.	*	.	.	*	*	.	.	*	.
45	.	.	*	.	.	*	*	.	.	*	.
47	.	.	*	.	.	*	*	.	.	*	.
49	.	.	*	.	.	*	*	.	.	*	.
51	.	.	*	.	.	*	*	.	.	*	.
53	.	.	*	.	.	.	*	.	.	*	.
55	.	.	.	.	.	.	*	.	.	.	.
57	.	.	.	.	.	.	*	.	.	.	.
59	.	.	.	.	.	.	.	.	.	.	.
61	.	.	.	.	.	.	.	.	.	.	.
63	.	.	.	.	.	.	.	.	.	.	.
65	.	.	.	.	.	.	.	.	.	.	.
67	.	.	.	.	.	.	.	.	.	.	.
69	.	.	.	.	.	.	.	.	.	.	.
71	.	.	.	.	.	.	.	.	.	.	.
73	.	.	.	.	.	.	.	.	.	.	.
75	.	.	.	.	.	.	.	.	.	.	.
77	.	.	.	.	.	*	.	.	.	.	.

* - inverse response
. - normal response

Table 7.10
Reflux Flow Rate After Time 0⁻

Test	% Change	New Reflux Flow Rate, mol/s
CL.RF.OL15	+5	27.75
CL.RF.OL16	-5	25.10
CL.RF.OL17	+10	29.07
CL.RF.OL18	-10	23.78

input rate, since both an increase in the reflux flow rate and a decrease in the heat input rate would effectively increase the reflux ratio. It was observed that the magnitude of variation in the reflux ratio is not in proportion to the magnitude of the corresponding disturbance. For example, increase in reflux flow rate of 10% will increase the reflux ratio much more than an increase of 5%, especially when the reflux ratio is high. It is possible that the nonlinear phenomenon, when the distillation unit is already operating at a high reflux ratio, is related to the highly nonlinear steady state gains in the stage temperatures and the compositions, as illustrated in Figures 7.17 and 7.18 for changes in the reflux flow rate. The inverse response maps in Tables 7.11 and 7.12 indicate that a few components exhibit inverse response behavior on a large number of stages for both an increase and decrease in reflux flow rate. However, no inverse response behavior in the stage temperatures can be observed.

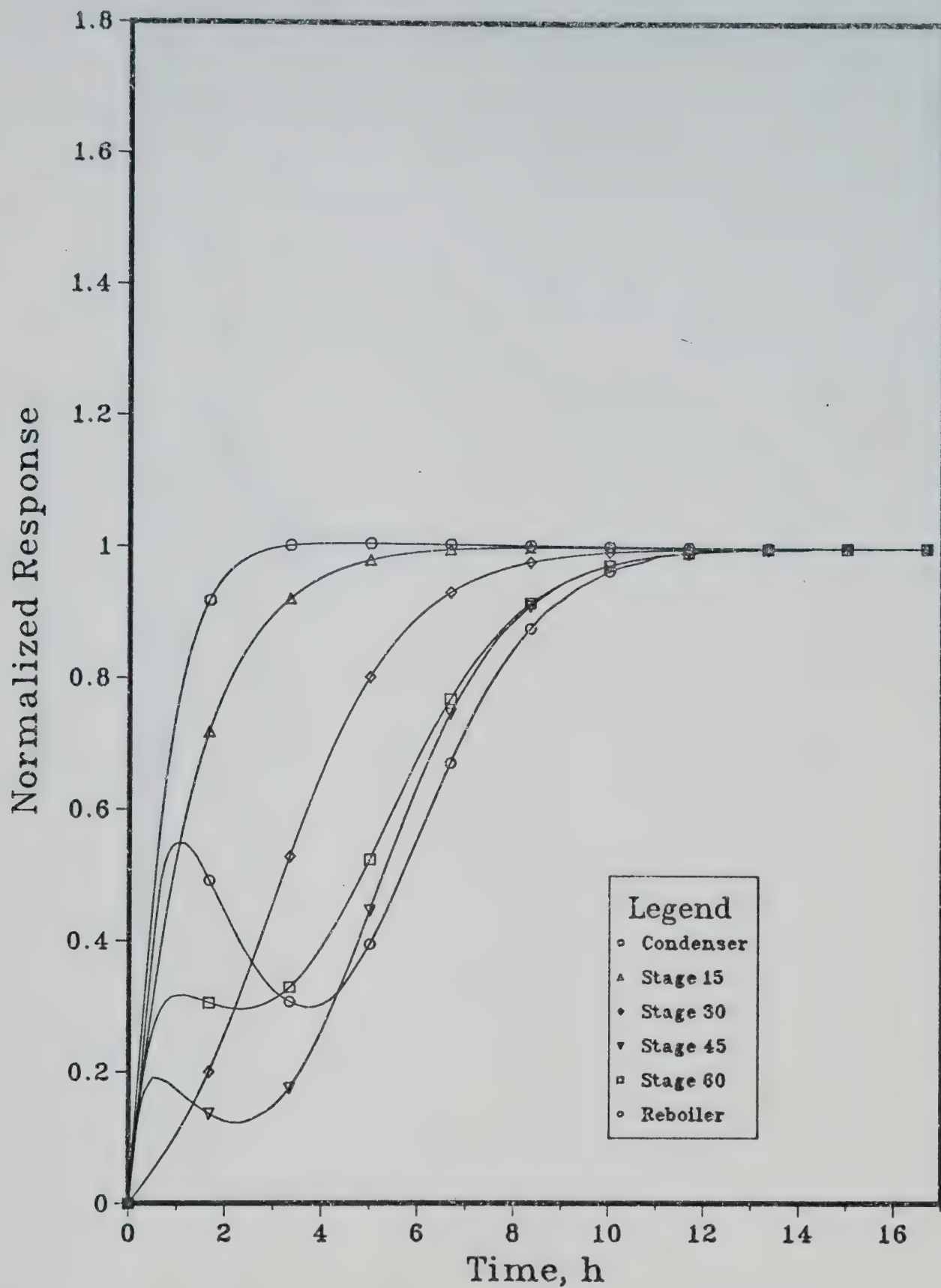


Fig. 7.13 Normalized Response of Stage Temperatures to a +5% Step Change in Reflux Flow Rate

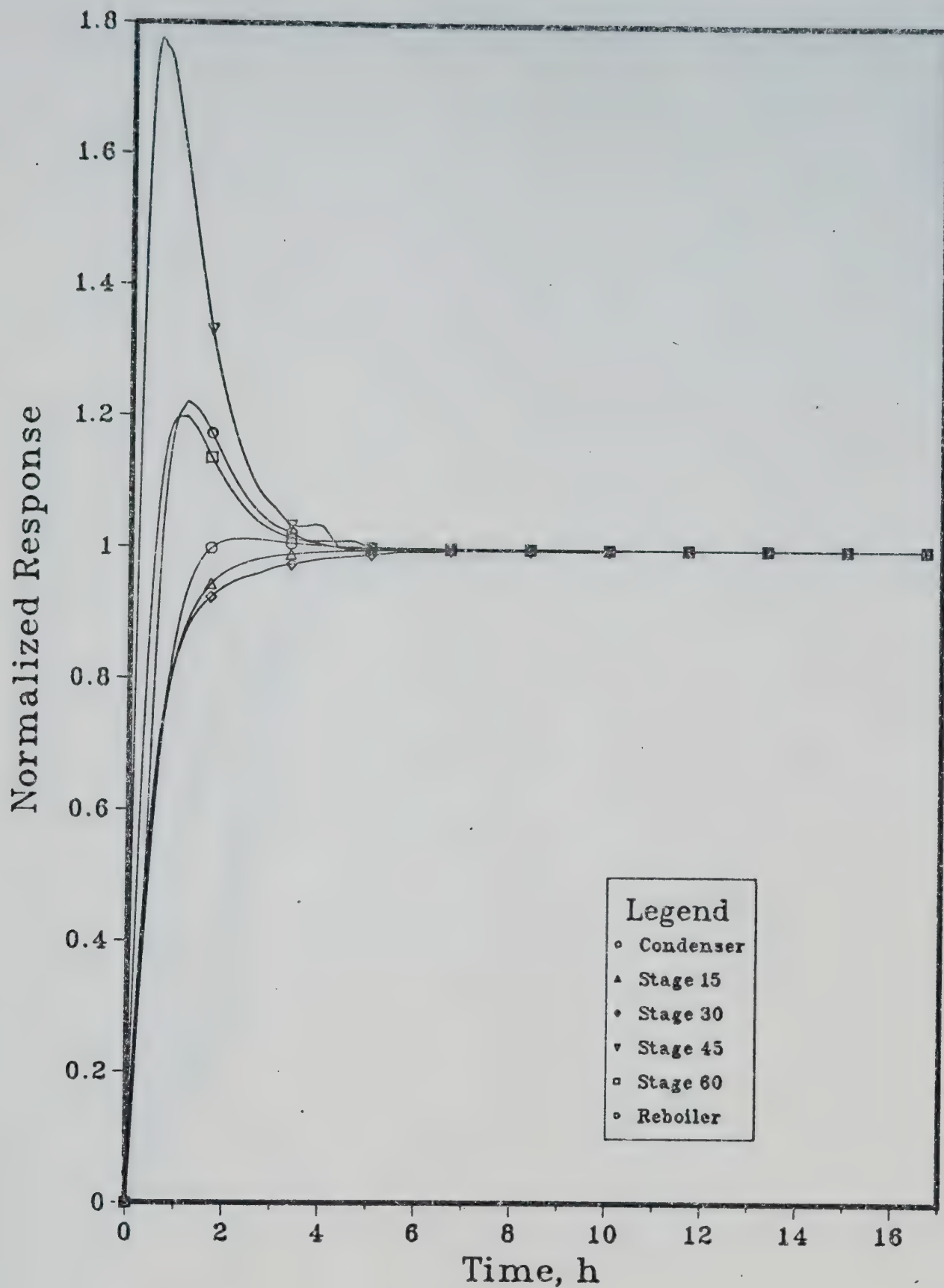


Fig. 7.14 Normalized Response of Stage Temperatures to a -5% Step Change in Reflux Flow Rate

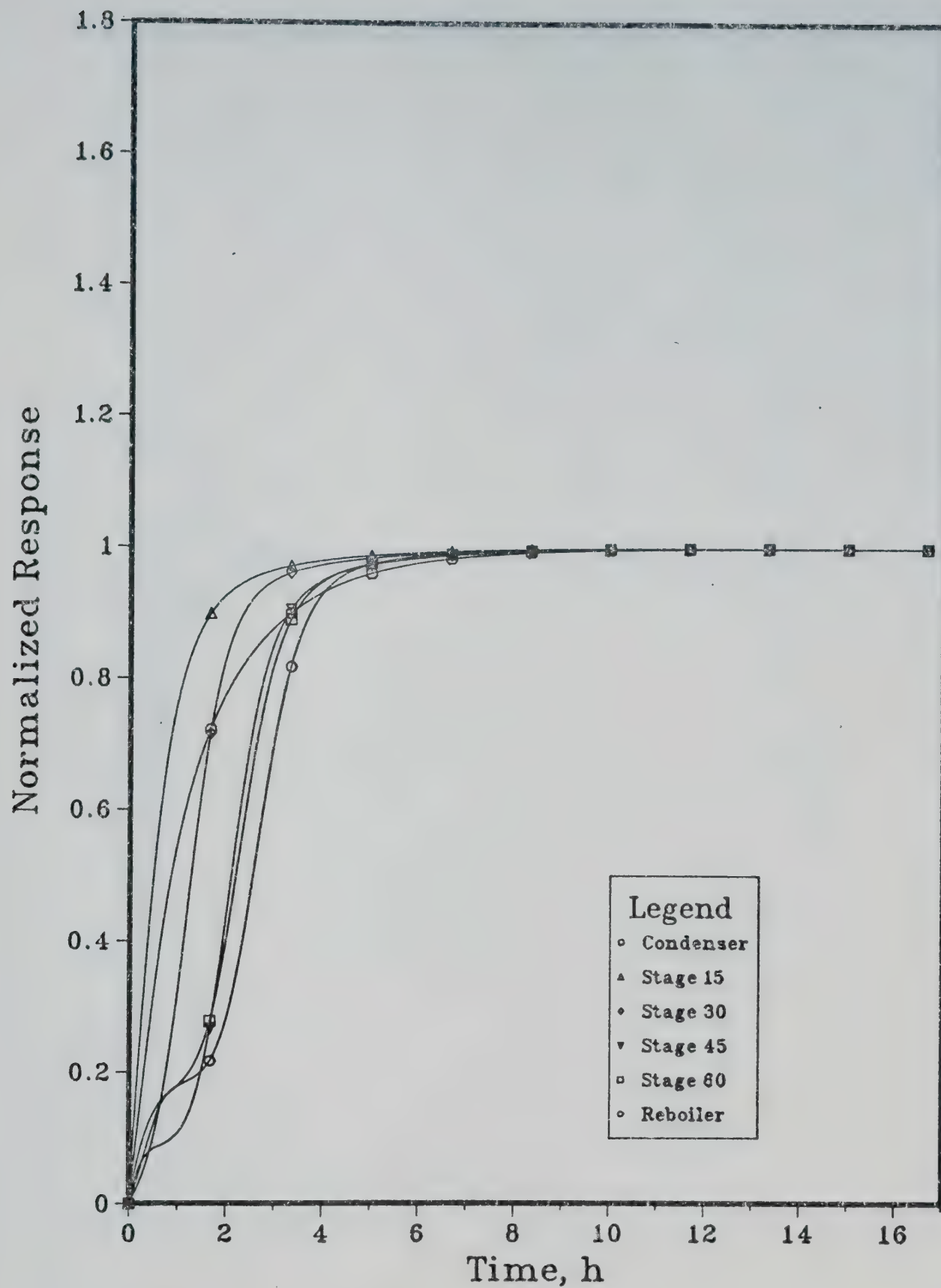


Fig. 7.15 Normalized Response of Stage Temperatures to a +10% Step Change in Reflux Flow Rate

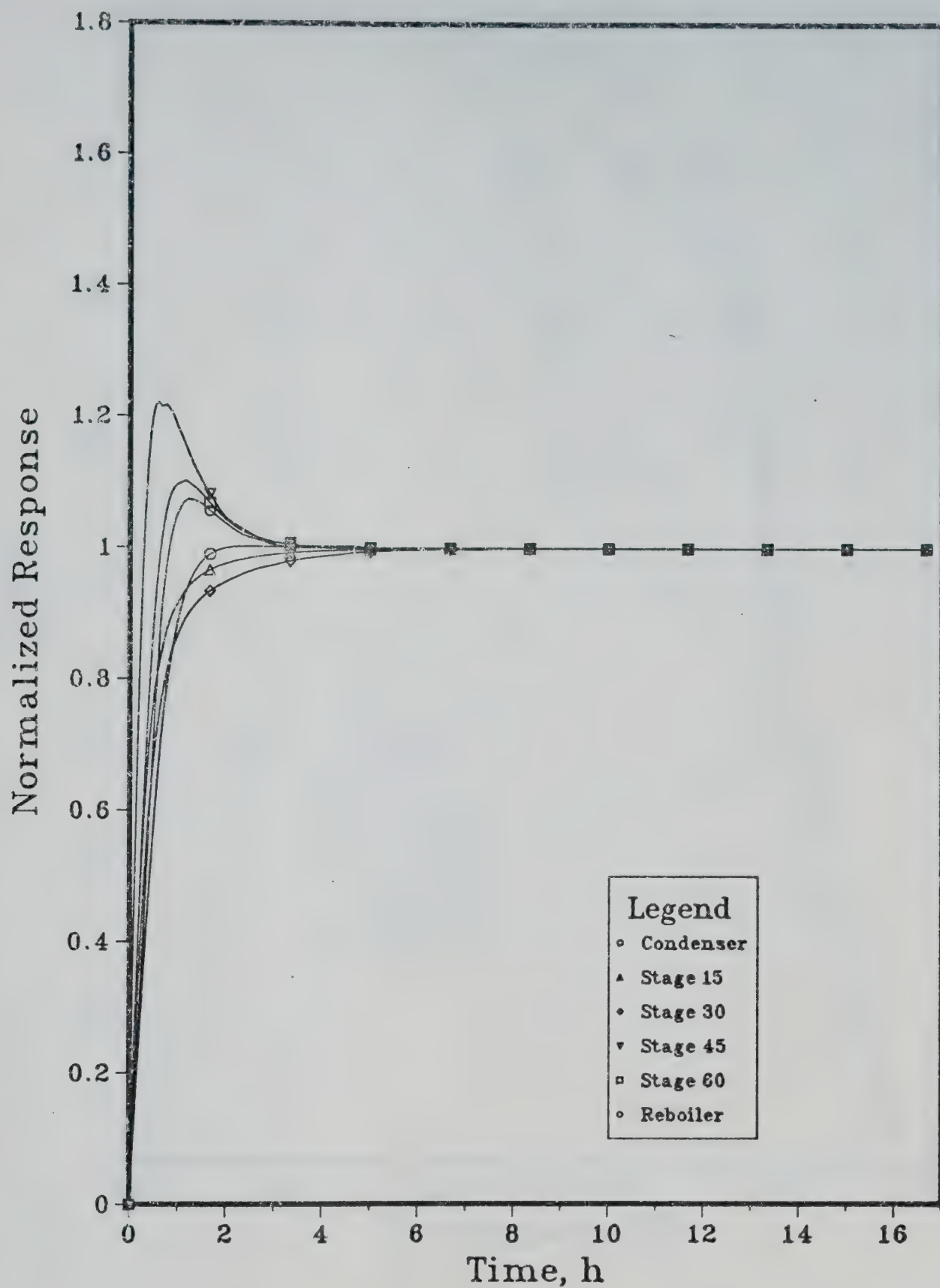


Fig. 7.16 Normalized Response of Stage Temperatures to a -10% Step Change in Reflux Flow Rate

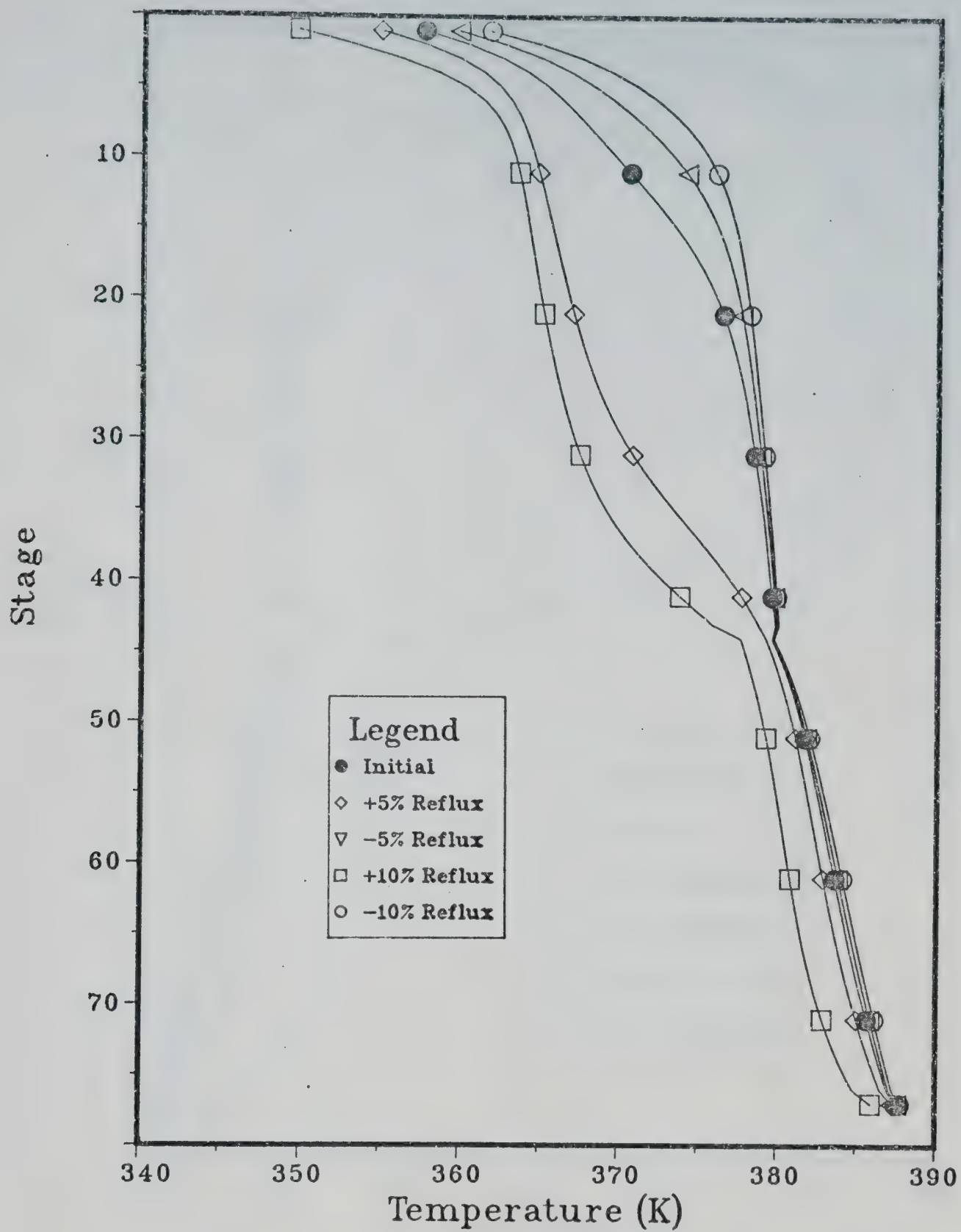


Fig. 7.17 Steady State Temperature Profiles for Changes in Reflux Flow Rate

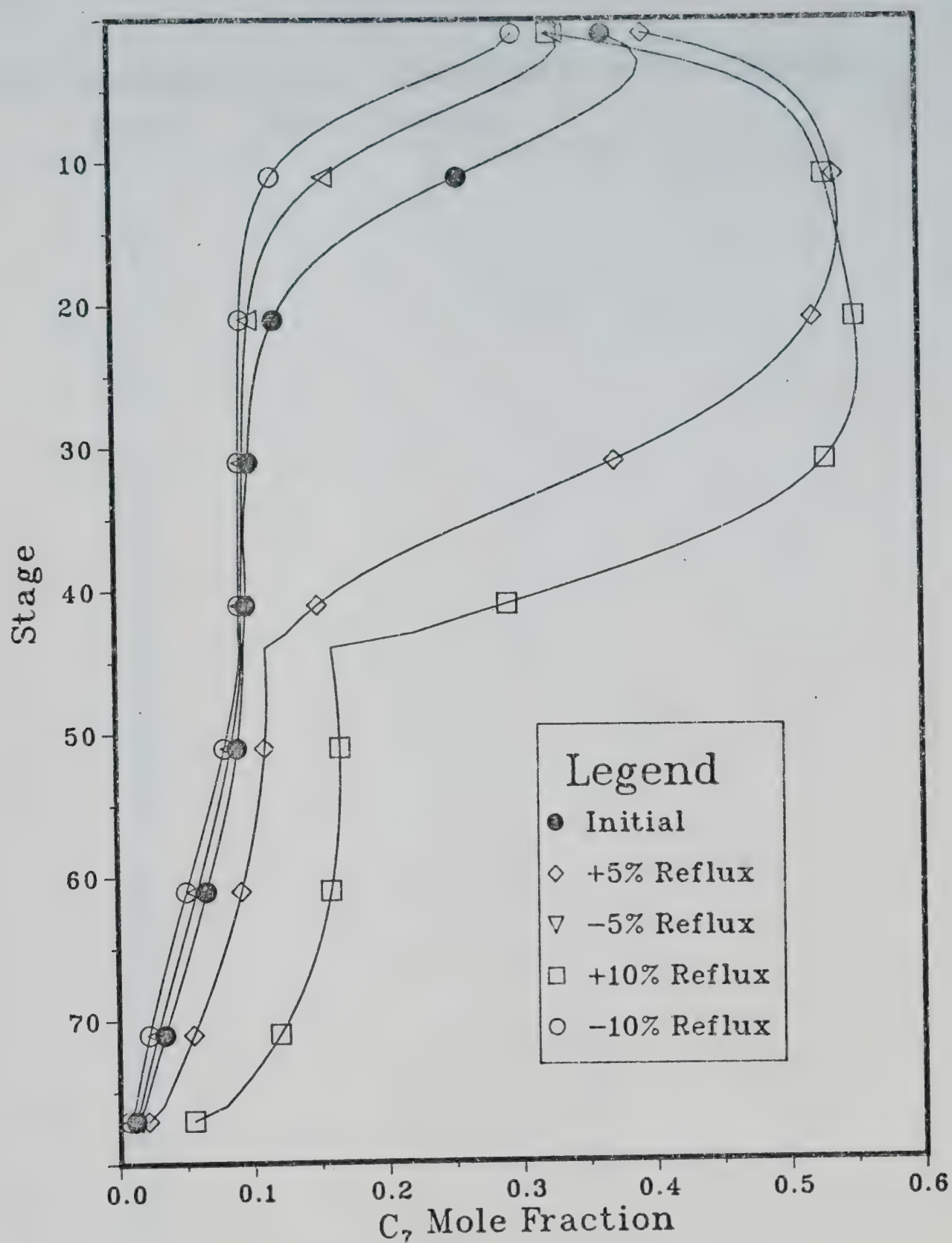


Fig. 7.18 Steady State C_7 Composition Profiles for Changes in Reflux Flow Rate

Table 7.11

Inverse Response Map for a +5% Change in Reflux Flow Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	*	.	.	.	.	*	.	.	*
3	.	.	.	.	.	.	.	.	.	.	.
5	.	.	.	.	.	.	*	.	.	.	.
7	.	.	.	.	.	.	.	.	.	.	.
9	.	.	.	.	.	.	.	.	.	.	.
11	.	.	.	.	.	.	.	.	.	.	.
13	.	.	.	.	.	.	.	.	.	.	.
15	.	.	.	.	.	.	.	.	.	.	.
17	.	.	.	.	.	.	.	.	.	.	.
19	.	.	.	.	.	.	.	.	.	.	.
21	.	.	.	.	.	.	.	.	.	*	.
23	.	.	.	.	.	.	.	.	.	*	.
25	.	.	.	.	.	*	.	.	.	*	.
27	.	.	.	.	.	*	.	.	.	*	.
29	.	.	.	.	.	*	.	.	.	*	.
31	.	.	.	.	*	*	.	.	.	*	.
33	.	.	.	.	*	*	.	.	.	*	.
35	.	.	*	.	*	*	.	.	.	*	.
37	.	.	*	.	.	*	.	.	.	*	.
39	.	.	.	.	.	*	.	.	.	*	.
41	.	.	.	.	.	*	*	.	.	.	.
43	.	.	.	.	.	*	*	.	.	.	.
45	.	.	*	.	.	*	*	.	.	.	.
47	.	.	*	.	.	*	*	.	.	.	.
49	.	.	*	.	.	*	*	.	.	.	.
51	.	.	*	.	.	*	*	.	.	*	.
53	.	.	.	.	.	*	*	.	.	*	.
55	.	.	.	.	.	*	*	.	.	*	.
57	.	.	.	.	.	*	.	.	.	*	.
59	.	.	.	.	.	*	.	.	.	*	.
61	.	.	.	.	.	*	.	.	.	*	.
63	.	.	.	.	.	*	.	.	.	*	.
65	.	.	.	.	.	*	.	.	.	*	.
67	.	.	.	.	.	*	.	.	.	.	.
69	.	.	.	.	.	*	.	.	.	.	.
71	.	.	.	.	.	*	.	.	.	*	.
73	.	.	.	.	.	*	.	.	.	.	.
75	.	.	.	*	.	*	.	.	.	.	.
77	.	.	.	.	.	*	.	.	.	.	.

* - inverse response

. - normal response

Table 7.12

Inverse Response Map for a -5% Change in Reflux Flow Rate

STAGE	TEMP	COMPONENT									
		1	2	3	4	5	6	7	8	9	10
1	.	.	.	.	.	.	*	.	.	.	.
3	.	.	.	.	.	.	.	.	.	.	.
5	.	.	.	.	.	.	.	.	.	.	.
7	.	.	.	.	.	.	.	.	.	.	.
9	.	.	.	.	.	.	.	.	.	.	.
11	.	.	.	.	.	.	.	.	.	*	.
13	.	.	.	.	.	.	.	.	.	*	.
15	.	.	.	.	*	.	.	.	.	*	.
17	.	.	.	.	*	.	.	.	.	.	.
19	.	.	.	.	*	*	.	.	.	.	.
21	.	.	.	.	*	.	.	.	.	.	.
23	.	.	.	.	*	.	.	.	.	.	.
25	.	.	.	.	*	.	.	.	.	.	.
27	.	.	.	.	*	.	.	.	.	.	.
29	.	.	.	.	*	.	.	.	.	.	.
31	.	.	.	.	*	.	.	.	.	.	.
33	.	.	.	.	*	.	.	.	.	.	.
35	.	*	.	.	*	.	*	.	.	.	.
37	.	.	.	.	*	.	*	.	.	.	.
39	.	.	*	.	*	.	.	.	.	.	.
41	.	.	.	.	*	.	.	.	.	.	.
43	.	.	*	.	.	.	.	.	.	.	.
45	.	.	.	.	*	.	*	.	.	.	.
47	.	.	.	.	.	.	.	.	.	.	.
49	.	.	.	.	*	.	*	.	.	.	.
51	.	.	.	.	*	.	.	.	.	.	.
53	.	.	.	.	.	.	.	.	.	.	.
55	.	.	.	.	*	.	.	.	.	.	.
57	.	.	.	.	.	.	.	.	.	.	.
59	.	.	.	.	.	*	.	.	.	.	.
61	.	.	.	.	.	*	.	.	.	*	.
63	.	.	.	.	*	*	.	.	.	*	.
65	.	.	.	.	.	*	.	.	.	.	.
67	.	.	.	.	*	*	.	.	.	.	.
69	.	.	.	.	*	*	.	.	.	.	.
71	.	.	.	.	.	*	.	.	.	.	.
73	.	.	.	.	.	.	.	.	.	.	.
75	.	.	.	.	.	.	.	.	.	.	.
77	.	.	.	.	.	.	.	.	.	.	.

* - inverse response
. - normal response

8. Conclusions and Recommendations

8.1 Conclusions and General Comments

1. By solving the distillation problems considered in the preceeding chapters, the distillation model has been demonstrated to be capable of providing accurate predictions of the steady state and the dynamic behavior for a wide range of columns. It was found that the variables in some columns are more sensitive to parameters such as heat input, heat loss, tray efficiencies and tray pressure drop than the variables of other columns. Therefore, unlike the approach used in some previous work, these parameters are allowed to be variable in the model. Furthermore, the assumption of constant tray holdup is removed so that the dynamic effects of the hydraulics can be modelled. The resulting model is a more accurate representation of the column behavior over a wide range of operating conditions.
2. The simulation software developed from the dynamic model has important features not available in some steady state or dynamic simulators which the author has access to. The simulator has a thermodynamic database to facilitate the simulation of any combination of components included, although more work may still be done in expanding this database to cover a wider range

of components. The simulation of the column can start from any user specified initial state and proceed to a final steady state, or the user may 'freeze' the simulation at any sample time to examine and plot all variables. Given sufficient information, the simulator can also calculate the steady state from a self-starting arbitrary initial state. Heat input, heat loss, tray efficiencies, pressure drop and tray holdups are all allowed to vary throughout the simulation. The simulator also allows a number of different disturbances to the column such as step changes in feed rates, feed properties, heat input rate and reflux rate.

3. The dynamic simulator has stronger stability and better performance compared to the simulator developed by Cook(30), who used a similar column model and a constant parameter semi-implicit Runge-Kutta method. The present simulator has no difficulty in solving the distillation problem in Chapter 4, which was originally solved by Cook(30). The simulator used by Cook occasionally aborts during execution for some column conditions. In contrast, this problem did not occur with the present simulator, although the range of column conditions was even wider.

The most significant improvement of the simulator over the other simulators used in this study, however, was its ability to simulate the 10 component industrial

separator in Chapter 7. The separator had been studied by some plant personnel and by the author, using private or commercial simulators, without much success in even reaching a steady state. However, both the steady state and the dynamic behavior have been simulated successfully using this simulator. The initial product compositions of the column were found to be close to the plant measurements. The dynamic response of the separator was also simulated, although no experimental data has been available for validation.

The simplified thermodynamic model used has shown to be accurate within the range of temperatures and pressures considered in the simulation study. The calculated results from the simplified model were compared with experimental data with good agreement. The simplified model was also compared with the results from a more rigorous model used by Gallun(13) who included vapor phase fugacities and enthalpy departure. The results shows that the simplified model is accurate in representing the mixture from which the experimental data were measured. The deviation of the results from the more rigorous model is negligible, yet the number of parameters and the amount of computation are reduced. Therefore, the simplified model is preferred over the more rigorous approach unless the columns being simulated have much higher pressures.

4. The Wilson equation has been used with much success

when applied to mixtures with a non-ideal liquid phase. It has demonstrated to be very useful in obtaining accurate results in cases where no specific equilibrium data are available from experiment. The ability of the Wilson equation in handling complex mixtures is illustrated in Chapter 7, in which the equation is applied to the 10 component mixture. In simulating this separator, difficulties in convergence had been encountered by other simulators. Although the convergence problem can be overcome by using a simple form of equilibrium representation on these simulators, large errors are found in the compositions of a few chemical species. On the other hand, The Wilson equation, when incorporated into the present simulator, successfully predicted the steady state compositions with good agreement with the plant data.

5. The comparison of the calculated response and the experimental data obtained from the pilot scale binary distillation column, indicated that the assumption of constant tray efficiency may not be valid when the column is subject to sufficiently large disturbances in feed flow rate. It was found that correlating the tray efficiency with a linear combination of the average vapor rate and the average liquid rate improves the agreement between the calculated and the measured response, although such an approach requires prior knowledge of the initial and the final steady state

conditions. Furthermore, the initial assumption that the overall heat transfer coefficient between the steam supplied to the reboiler and the process liquid is constant had to be removed. The final results indicated that correlating the overall heat transfer coefficient as a function of the temperature of the process liquid, using a constant empirical parameter, yielded more accurate results over the range of column conditions than with the assumption of constant heat transfer.

6. The results obtained from this simulation study indicate that distillation columns often exhibit nonminimum phase response behavior and highly nonlinear characteristics. The column models that exhibit such behavior ranged from a simplified model with hydrocarbon components, to a complex distillation model with a highly non-ideal liquid mixture. Although such column behavior has not been confirmed by experiment, the potential control problems can be serious. Being able to predict column behavior over a wide range of operating conditions, the dynamic simulator can be used to help discover potential control problems even before the column design is completed. Furthermore, if reliable parameters for a particular column are available, the simulator can be utilized to calculate the transfer functions needed for control analyses. This work is an attempt to improve the science of

column simulation, so that column control problems can be solved using a minimal amount of experimental work.

7. The ASIRK integration method is relatively easy to use for solving the large set of ordinary differential equations in column simulation, although the algorithm is slightly more complicated than the constant parameter semi-implicit Runge-Kutta methods. For solving distillation problems, the ASIRK has been demonstrated to be more efficient than the constant parameter semi-implicit method developed by Ballard et al(11). The method also has the advantage that memory requirement is smaller, since this one-step algorithm does not require storage of past values as in other multi-step algorithms such as Gear's method. Moreover, the method is geared for accurate tracking of stiff variables since the parameters are adjusted based on the eigenvalues of the stiff variables. Therefore the ASIRK integration method is highly recommended for use in column simulation and other calculations involving large sets of stiff differential equations.

8.2 Recommendations for Future Work

Development of the digital simulator used in this work into a general purpose program is still in the preliminary stage, and the validation tests have been limited to just a few cases. Future development of the simulator should lie in the following areas

1. More study of the phase equilibrium model is necessary in order to improve the prediction of the phase equilibria for systems such as that of the 10 component industrial distillation column discussed in Chapter 7. Since the mixture probably has one or more azeotropes, it may become necessary to use equation of states which can predict azeotropes, and to perform equilibria experiments to obtain the needed parameters. Furthermore, it is desirable to incorporate more than one thermodynamic model into the dynamic simulator to provide the user with a broader choice of thermodynamic models.
2. Detailed modelling of the condenser and the reboiler may be necessary. Although the condenser and reboiler models can be conveniently derived from the basic tray model, this may not provide adequate representations of the dynamic behavior of the units. For example, if these units have large holdups, the assumption of perfect mixing may not be valid. The heat transfer process in these units may also have important dynamic effect on the overall characteristics of the column.
3. Extension of the dynamic simulator for the simulation of trains of multicomponent distillation columns since the current version of the dynamic simulator can only simulate a single column. This is particularly important since separation operations, designed for energy integration, employ multiple columns.

4. A more "user friendly" interface for easy utilization of the dynamic simulator by inexperienced users should be developed. This interface would transform simulation specifications and parameters into a data file suitable for computer input. The importance of such an enhancement becomes obvious if the dynamic simulator is to be extended to include multicolumn configurations. One possible approach is the development of an interactive program to prompt for all necessary input parameters from the user, and construct the input data file automatically. The program could be menu driven such that the user can easily choose from a variety of model options, and the program would prompt for the pertinent parameters for the particular option chosen. This approach offers the advantage that the user, if ever in doubt, can be assisted any time during the execution of the program so that the construction of the input data file becomes a relatively easy task and input errors are minimized.

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Appendix A - Derivation of Model Equations

A.1 Derivation of Tray Component Balance Equation, equation 2.2

The component balance of the component i on the stage j is given as

$$\begin{aligned} d[M_j x_j]/dt = & \{F_j z_j + V_{j+1} y_{j+1} + L_{j-1} x_{j-1} \\ & - (V_j + S_j) y_j - (L_j + s_j) x_j\} \end{aligned} \quad (A.1)$$

Expanding the left hand side of the above equation yields

$$d[M_j x_j] = x_j [dM_j/dt] + M_j [dx_j/dt] \quad (A.2)$$

The $d[M_j/dt]$ term in equation A.2 can be replaced by use of equation 2.1, expressed as

$$dM_j/dt = F_j + V_{j+1} + L_{j-1} - (V_j + S_j) - (L_j + s_j) \quad (2.1)$$

After this substitution and equating equations A.1 and A.2, equation 2.2 in Chapter 2 results

$$\begin{aligned} dx_j/dt = & \{F_j (z_j - x_j) + V_{j+1} (y_{j+1} - x_j) \\ & + L_{j-1} (x_{j-1} - x_j) - (V_j + S_j) (y_j - x_j)\} / M_j \end{aligned} \quad (2.2)$$

A.2 Derivation of Energy Balance Equation, Equation 2.5

The balance equation for the total energy on the j th stage, equation 2.3, is

$$\begin{aligned} d[M_j h_j]/dt = \{ F_j(h_{f,j}) + Q_j + V_{j+1}H_{j+1} + L_{j-1}h_{j-1} \\ - (V_j + S_j)H_j - (L_j + s_j)h_j \} \end{aligned} \quad (2.3)$$

Now expanding the left hand side yields

$$d[M_j h_j] = h_j [dM_j/dt] + M_j [dh_j/dt] \quad (A.3)$$

Substituting equation 2.1 into the first term on the right hand side of equation A.3, and equating equation 2.3 with equation A.3 results in the differential form of the energy balance

$$\begin{aligned} dh_j/dt = \{ [F_j(h_{f,j} - h_j)] + Q_j + V_{j+1}(H_{j+1} - h_j) \\ + L_{j-1}(h_{j-1} - h_j) - (V_j + S_j)(H_j - h_j) \} / M_j \end{aligned} \quad (2.4)$$

The next step is to transform equation 2.4 into an algebraic equation. Since the liquid on the stage is assumed to be at the equilibrium temperature, the enthalpy is therefore a function of time and the equilibrium composition. Assuming the pressure effect on the liquid enthalpy is negligible, the left hand side of equation 2.4 can be expanded as

$$\begin{aligned} dh_j/dt = \left[\frac{\partial h_j}{\partial T_j} \right] \cdot \left[\frac{dT_j}{dt} \right] + \sum_i \left[\frac{\partial h_j}{\partial x_{j,i}} \cdot \frac{dx_{j,i}}{dt} \right] \quad (A.4) \\ i=1, 2, \dots, C \end{aligned}$$

Also, the variation of the equilibrium temperature can be written as

$$\frac{dT_j}{dt} = \sum_i \left[\frac{\partial T_j}{\partial x_{ji}} \cdot \frac{dx_{ji}}{dt} \right] \quad i=1,2,\dots,C \quad (A.5)$$

Substitution of equation A.5 into equation A.4 and replacement of $\partial h_j / \partial T_j$ by C_{p_j} , the constant pressure heat capacity, yields

$$\frac{dh_j}{dt} = \sum_i \left[C_{p_j} \frac{\partial T_j}{\partial x_{ji}} + \frac{\partial h_j}{\partial x_{ji}} \right] \frac{dx_{ji}}{dt} \quad i=1,2,\dots,C \quad (A.6)$$

To simplify the appearance of the equations, let

$$\Gamma_{ji} = C_{p_j} (\partial T_j / \partial x_{ji}) + (\partial h_j / \partial x_{ji}) \quad (A.7)$$

After replacing dx_{ji}/dt in equation A.6 by the composition balance in equation 2.2, the following equation is obtained

$$\begin{aligned} dh_j/dt = \{ & F_j \sum_i [\Gamma_{ji} (z_{ji} - x_{ji})] + V_{j+1} \sum_i [\Gamma_{ji} (y_{j+1,i} - x_{ji})] + \\ & L_{j-1} \sum_i [\Gamma_{ji} (x_{j-1,i} - x_{ji})] - (V_j + S_j) \sum_i [\Gamma_{ji} (y_{ji} - x_{ji})] \} / M_j \end{aligned} \quad (A.8)$$

Note that all terms involving L_j are eliminated by the manipulation.

For the purpose of simplicity, the following terms, without any physical interpretation, are defined

$$\xi_j = \sum_i [\Gamma_{ji} (x_{j-1,i} - x_{ji})]$$

$$\begin{aligned}
\xi_j^1 &= \sum_i [\Gamma_{ji}(y_{ji} - x_{ji})] \\
\xi_j^2 &= \sum_i [\Gamma_{ji}(y_{j+1,i} - x_{ji})] \\
\xi_j^3 &= \sum_i [\Gamma_{ji}(z_{ji} - x_{ji})] \quad i=1,2,\dots,C \quad (A.9)
\end{aligned}$$

Using these terms in equation A.8, the equation can be equated to equation 2.4 to eliminate the derivative term, that is

$$\begin{aligned}
\{F_j \xi_j^1 + Q_j + V_{j+1} \xi_j^2 + L_{j-1} \xi_j^3 - (V_j + S_j) \xi_j^2\} \\
= F_j(h_{t,j} - h_j) + Q_j + V_{j+1}(H_{j+1} - h_j) \\
+ L_{j-1}(h_{j-1} - h_j) - (V_j + S_j)(H_j - h_j)
\end{aligned}$$

which can be rearranged as

$$\begin{aligned}
F_j(h_{t,j} - h_j - \xi_j^1) + Q_j - S_j(H_j - h_j - \xi_j^2) \\
= V_j(H_j - h_j - \xi_j^2) - L_{j-1}(h_{j-1} - h_j - \xi_j^3) - V_{j+1}(H_{j+1} - h_j - \xi_{j+1}^2) \quad (A.10)
\end{aligned}$$

To further simplify the equation, let

$$a_j = h_{t,j} - h_j - \xi_j^1$$

$$\beta_j = H_j - h_j - \xi_j^2$$

$$\psi_j = H_{j+1} - h_j - \xi_j^3$$

and
$$E_j = F_j(h_{t,j} - h_j - \xi_j^1) - \beta_j S_j + Q_j$$

Using the above definitions in equation A.10, equation 2.5 is readily obtained

$$E_j = -a_j L_{j-1} + \beta_j V_j - \psi_j V_{j+1} \quad (2.5)$$

A.3 Method of Solution for the Liquid and Vapor Flow Rates

A.3.1 Case 1: Constant Molar Holdup

The mass balance equation and the energy balance equation are rewritten here as follows

$$m_j = L_{j-1} - L_j - V_j + V_{j+1} \quad (2.14)$$

$$E_j = -\alpha_j L_{j-1} + \beta_j V_j - \psi_j V_{j+1} \quad (2.5)$$

Two methods can be used to solved for L_j and V_j . The first method is the Gauss-Seidel iterative method which requires the above equation to be explicit in L_j and V_j . For example, applying the end conditions for a total condenser and a partial reboiler yields

$$L_1 = V_2 - m_1$$

$$V_1 = 0 \quad (\text{total condenser})$$

$$L_j = L_{j-1} - V_j + V_{j+1} - m_j$$

$$V_j = (\alpha_j L_{j-1} + \psi_j V_{j+1} + E_j) / \beta_j \quad j=2, \dots, n-1$$

$$L_n = L_{n-1} - V_n - m_n$$

$$V_n = (\alpha_n L_{n-1} + E_n) / \beta_n \quad (\text{partial reboiler})$$

This method also requires a reasonable initial estimate of L_j and V_j in order to have satisfactory convergence rate. However, this is not a problem in most cases since the liquid and vapor flow rates from the last time step can be use as the initial estimate.

A more direct method discussed by Brosilow et al(13) takes the following steps

- i. Multiply equation 2.14 by ψ_j and add the result to equation 2.5 to eliminate V_{j+1} , giving

$$V_j = \frac{\psi_j - a_j}{\psi_j - \beta_j} L_{j-1} - \frac{\psi_j}{\psi_j - \beta_j} L_j - \frac{(\psi_j m_j + E_j)}{\psi_j - \beta_j} \quad (\text{A.11})$$

- ii. Substitute the expression for V_j with dummy index j and $j+1$ into equation 2.14 to obtain the following form of equation

$$A_j L_{j-1} - B_j L_j + C_j L_{j+1} = D_j \quad (\text{A.12})$$

where A_j , B_j , C_j and D_j are defined as follows

$$\begin{aligned} A_j &= 1 - \frac{\psi_j - a_j}{\psi_j - \beta_j} \\ B_j &= 1 - \frac{\psi_j}{\psi_j - a_j} - \frac{(\psi_{j+1} - a_{j+1})}{(\psi_{j+1} - \beta_{j+1})} \\ C_j &= - \frac{\psi_{j+1}}{\psi_{j+1} - \beta_{j+1}} \\ D_j &= m_j - \frac{(E_j + \psi_j m_j)}{\psi_j - \beta_j} + \frac{(E_{j+1} + \psi_j m_{j+1})}{\psi_{j+1} - \beta_{j+1}} \end{aligned}$$

- iii. Set up a tridiagonal system of equations based on equation A.12 and solve for the liquid flow rates.
- iv. Solve the vapor flow rates with equation 2.5 using the resulting liquid flow rates from step iii.

A.3.2 Case 2: Tray Holdup as a Function of Liquid Flow Rate

In this method of solution, it is assumed that the liquid flow rates have already been solved by integrating the tray hydraulics equation 2.18. The remaining task is to solve the vapor flow rates based on the liquid flow rates. In principle, the mass balance equation is already used in solving the tray hydraulic equations, therefore the energy balance equations are necessarily used for the vapor flow rate calculations.

Starting from the reboiler stage, where equation 2.5 can be written as

$$V_n = (E_n + a_n L_{n-1}) / \beta_n \quad (\text{partial reboiler})$$

The remaining vapor flow rates are solved backwards from stage $n-1$, ie.

$$V_j = (a_j L_{j-1} + \psi_j V_{j+1} + E_j) / \beta_j \quad j=n-1, \dots, 2$$

$$\text{and} \quad V_1 = 0 \quad (\text{total condenser})$$

A.4 Derivation of the Weir Equation, Equation 2.15

The Francis weir formula(14) is given as

$$q_j/W = 1.839 (h_e)^{3/2} \quad (\text{A.13})$$

with q_j in m^3/sec , W and h_e in metres.

Rearranging equation A.13 with time units expressed in

minutes gives

$$h_t = 0.04347 (q_j/W)^{2/3}$$

And since $q_j = L_j v_j$

where v_j is the molar volume of the mixture in kmol/m^3 , the following expression is obtained

$$h_t = 0.04347 (L_j v_j / W)^{2/3}$$

An expression for the molar holdup is then obtained as follows

$$M_j = [(h_t + hw) A_t / v_j] (1 - \epsilon) \quad (\text{A.14})$$

with A_t expressed in m^2 , and hw in metres.

Substitution of the expression for h_t into equation A.14 yields

$$M_j = \{0.04347 [L_j v_j / W]^{2/3} + hw\} A_t (1 - \epsilon) / v_j \quad (2.15)$$

Now differentiation with respect to L_j gives

$$\frac{dM_j}{dL_j} = \left\{ \frac{0.02898 A_t (1 - \epsilon)}{W} \right\} \left\{ \frac{L_j v_j}{W} \right\}^{-1/3} \quad (\text{A.15})$$

or

$$\frac{dL_j}{dM_j} = \left\{ \frac{W}{0.02898 A_t (1 - \epsilon)} \right\} \left\{ \frac{W}{L_j v_j} \right\}^{-1/3}$$

which is equation 2.16.

Appendix B - Thermodynamic Parameters

Thermodynamic Parameters for Chapter 3

Table B3.1
Equilibrium Data(33) at $P = 300\text{lb/in}^2$

$$(K_i/T)^{1/3} = a_{1i} + a_{2i}T + a_{3i}T^2 + a_{4i}T^3 \quad (T \text{ in } R)$$

Component	$a_{1i} \cdot 10^2$	$a_{2i} \cdot 10^5$	$a_{3i} \cdot 10^8$	$a_{4i} \cdot 10^{12}$
C_3H_8	-14.512474	53.638924	-5.3051604	-173.58329
$n-C_4H_{10}$	-14.181715	36.866353	16.521412	-248.23843
$n-C_6H_{14}$	1.1506919	-33.885839	97.795401	-542.35941

Table B3.2
Liquid Enthalpy Data(34) at $P = 300\text{lb/in}^2$

$$(h_i)^{1/2} = c_{1i} + c_{2i}T + c_{3i}T^2 \quad (T \text{ in } R)$$

Component	c_{1i}	$c_{2i} \cdot 10^1$	$c_{3i} \cdot 10^5$
C_3H_8	-14.50006	1.9802223	-2.9048837
$n-C_4H_{10}$	-20.29811	2.3005743	-3.8663417
$n-C_6H_{14}$	-23.87041	2.6768089	-4.4197793

Table B3.3
Vapor Enthalpy Data(34) at $P = 300\text{lb/in}^2$

$$(H_i)^{1/2} = e_{1i} + e_{2i}T + e_{3i}T^2 \quad (T \text{ in } R)$$

Component	e_{1i}	$e_{2i} \cdot 10^4$	$e_{3i} \cdot 10^6$
C_3H_8	81.795910	389.81919	36.470900
$n-C_4H_{10}$	152.66798	-1153.4842	146.64125
$n-C_6H_{14}$	85.834950	1552.3917	-34.018595

Thermodynamic Parameters for Chapter 4

Table B4.1
Equilibrium Data(11)

$$K_i = \exp\{a_{1i} + a_{2i}/T + a_{3i}/T^2\} \quad (T \text{ in K})$$

Component	a_{1i}	a_{2i}	a_{3i}
Ethane	0.649086E+00	0.421544E+04	-0.882222E+06
Propylene	0.391245E+01	0.186111E+04	-0.533920E+06
Propane	0.384851E+01	0.192822E+04	-0.560525E+06
Iso-butane	0.684489E+01	-0.167722E+03	-0.252485E+06
Cis-butene-2	0.658149E+01	0.174340E+02	-0.317562E+06

Table B4.2
Liquid Enthalpy Data(11)

$$h_i = c_{1i} + c_{2i}T \quad (T \text{ in K, } h_i \text{ in kJ/kmol})$$

Component	c_{1i}	c_{2i}
Ethane	-3.050700	0.040113
Propylene	-3.507600	0.045986
Propane	-5.480700	0.053833
Iso-butane	-7.743300	0.038080
Cis-butene-2	-3.899100	0.059589

Table B4.3
Vapor Enthalpy Data(11)

$$H_i = e_{1,i} + e_{2,i}T + e_{3,i}T^2 \quad (T \text{ in K, } H_i \text{ in kJ/kmol})$$

Component	$e_{1,i}$	$e_{2,i}$	$e_{3,i}$
Ethane	0.684620E+01	0.199386E-01	-0.422788E-05
Propylene	0.966230E+01	0.185670E-01	0.626584E-05
Propane	0.105420E+02	0.138070E-01	0.206430E-04
Iso-butane	0.134260E+02	0.947720E-02	0.436136E-04
Cis-butene-2	0.173470E+02	0.226330E-02	0.448513E-04

Thermodynamic Parameters for Chapter 5

Table B5.1
Wilson Interaction Energy

Component	$a_{ij}, \text{cal/mol}$	
	H ₂ O	CH ₃ OH
H ₂ O	0.0	590.19
CH ₃ OH	-164.98	0.0

Table B5.2
Molar Volume and Antoine Coefficients

$$P_i^s = A_i - B_i / (T + C_i) \quad (T \text{ in K, } P_i^s \text{ in mmHg})$$

Component	v_i l/kmol	A_i	B_i	C_i
H ₂ O	18.02	18.3036	3816.44	-46.13
CH ₃ OH	40.73	18.5875	3626.55	-34.29

Table B5.3
Liquid Enthalpy Data

$$h_i = c_{1i} + c_{2i}T + c_{3i}T^2 + c_{4i}T^3 + c_{5i}T^4$$

(T in K, h_i in kJ/kmol)

Comp.	c_{1i}	c_{2i}	$c_{3i} \cdot 10^2$	$c_{4i} \cdot 10^4$	$c_{5i} \cdot 10^8$
H ₂ O	-26972.	147.05	-29.533	5.2676	-34.028
CH ₃ OH	-58200.	577.65	-241.74	48.868	-337.9

Table B5.4
Vapor Enthalpy Data

$$H_i = e_{1,i} + e_{2,i}T + e_{3,i}T^2 + e_{4,i}T^3 + e_{5,i}T^4$$

(T in K, H_i in kJ/kmol)

Comp.	$e_{1,i}$	$e_{2,i}$	$e_{3,i} \cdot 10^2$	$e_{4,i} \cdot 10^4$	$e_{5,i} \cdot 10^6$
H ₂ O	31716.	32.221	0.096128	0.035160	-0.089851
CH ₃ OH	26700.	21.1376	3.54385	0.086176	-0.71243

Thermodynamic Parameters for Chapter 6

Table B6.1
Wilson Interaction Energy

Component	$a_{ij}, \text{cal/mol}$			
	1	2	3	4
1	0.0	603.93	135.08	-164.98
2	-186.40	0.0	174.57	-23.32
3	-132.10	253.31	0.0	339.19
4	590.19	1549.3	881.11	0.0

1 - Methanol, 2 - Acetone, 3 - Ethanol, 4 - Water

Table B6.2
Molar Volume and Antoine Coefficients

$$P_i^s = A_i - B_i / (T + C_i) \quad (T \text{ in K, } P_i^s \text{ in mmHg})$$

Component	v_i l/kmol	A_i	B_i	C_i
1	40.73	18.5875	3626.55	-34.29
2	74.05	16.6513	2940.46	-35.93
3	58.68	18.9119	3803.98	-41.68
4	18.02	18.3036	3816.44	-46.13

Table B6.3
Liquid Enthalpy Data

$$h_i = c_{1i} + c_{2i}T + c_{3i}T^2 + c_{4i}T^3 + c_{5i}T^4$$

(T in K, h_i in kJ/kmol)

Comp.	c_{1i}	c_{2i}	$c_{3i} \cdot 10^2$	$c_{4i} \cdot 10^4$	$c_{5i} \cdot 10^8$
1	-58200.	577.65	-241.74	48.868	-337.9
2	-38428.	206.70	-46.095	9.5974	-57.47
3	-38670.	317.85	-128.73	28.738	-191.70
4	-26972.	147.05	-29.533	5.2676	-34.028

Table B6.4
Vapor Enthalpy Data

$$H_i = e_{1i} + e_{2i}T + e_{3i}T^2 + e_{4i}T^3 + e_{5i}T^4$$

(T in K, H_i in kJ/kmol)

Comp.	e_{1i}	e_{2i}	$e_{3i} \cdot 10^2$	$e_{4i} \cdot 10^4$	$e_{5i} \cdot 10^8$
1	26700.	21.1376	3.54385	0.086176	-0.71243
2	18508.	6.29692	13.0206	-0.417283	0.509088
3	28870.	9.00815	10.6964	-0.279491	0.034309
4	31716.	32.221	0.096128	0.035160	-0.089851

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